

Julian Avila, Trent Hauck

scikit-learn Cookbook

Second Edition

Over 80 recipes for machine learning in Python
with scikit-learn



Packt>

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Over 80 recipes for machine learning in Python
with scikit-learn

Julian Avila
Trent Hauck



BIRMINGHAM - MUMBAI

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He started programming in middle school, including games and geometrically artistic animations. He competed successfully in math and programming and worked for several groups at MIT. Julian has written complete software projects in elegant Python with just-in-time compilation. Some memorable projects of his include a large-scale facial recognition system for videos with neural networks on GPUs, recognizing parts of neurons within pictures, and stock market trading programs.

I would like to thank most of all my wife, Karen, for her immense support while writing this book. I would like to thank my daughters, Annelise and Sofia. Annelise considers this her book. I am very grateful to Bo Morgan who suggested I use scikit-learn many years ago. We had many artificial intelligence discussions and Bo introduced me to Marvin Minsky's layers of mental activities and neural networks. I would like to thank as well the late Marvin, who was Bo's advisor. I am grateful to Jose Ramirez, co-founder of Ayaakua, where I applied neural networks and machine learning with scikit-learn to computer vision problems.

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Oleg currently lives and works in Hamburg, Germany.

I would like to express my deepest gratitude to my parents for everything that they have done for me.

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Preface

Starting with installing and setting up scikit-learn, this book contains highly practical recipes on common supervised and unsupervised machine learning concepts. Acquire your data for analysis; select the necessary features for your model; and implement popular techniques such as linear models, classification, regression, clustering, and more in no time at all! The book also contains recipes on evaluating and fine-tuning the performance of your model. The recipes contain both the underlying motivations and theory for trying a technique, plus all the code in detail.

"Premature optimization is the root of all evil"

- Donald Knuth

scikit-learn and Python allow fast prototyping, which is in a sense the opposite of Donald Knuth's premature optimization. Personally, scikit-learn has allowed me to prototype what I once thought was impossible, including large-scale facial recognition systems and stock market trading simulations. You can gain instant insights and build prototypes with scikit-learn. Data science is, by definition, scientific and has many failed hypotheses. Thankfully, with scikit-learn you can see what works (and what does not) within the next few minutes.

Additionally, Jupyter (IPython) notebooks feature a nice interface that is very welcoming to beginners and experts alike and encourages a new scientific software engineering mindset. This welcoming nature is refreshing because, in innovation, we are all beginners.

In the last chapter of this book, you can make your own estimator and Python transitions from a scripting language to more of an object-oriented language. The Python data science ecosystem has the basic components for you to make your own unique style and contribute heavily to the data science team and artificial intelligence.

In analogous fashion, algorithms work as a team in the stacker. Diverse algorithms of different styles vote to make better predictions. Some make better choices than others, but as long as the algorithms are different, the choice in the end will be the best. Stackers and blenders came to prominence in the Netflix \$1 million prize competition won by the team Pragmatic Chaos.

Welcome to the world of scikit-learn: a very powerful, simple, and expressive machine learning library. I am truly excited to see what you come up with.

What this book covers

Chapter 1, *High-Performance Machine Learning – NumPy*, features your first machine learning algorithm with support vector machines. We distinguish between classification (what type?) and regression (how much?). We predict an outcome on data we have not seen.

Chapter 2, *Pre-Model Workflow and Pre-Processing*, exposes a realistic industrial setting with plenty of data munging and pre-processing. To do machine learning, you need good data, and this chapter tells you how to get it and get it into good form for machine learning.

Chapter 3, *Dimensionality Reduction*, discusses reducing the number of features to simplify machine learning and allow better use of computational resources.

Chapter 4, *Linear Models with scikit-learn*, tells the story of linear regression, the oldest predictive model, from the machine learning and artificial intelligence lenses. You deal with correlated features with ridge regression, eliminate related features with LASSO and cross-validation, or eliminate outliers with robust median-based regression.

Chapter 5, *Linear Models – Logistic Regression*, examines the important healthcare datasets for cancer and diabetes with logistic regression. This model highlights both similarities and differences between regression and classification, the two types of supervised learning.

Chapter 6, *Building Models with Distance Metrics*, places points in your familiar Euclidean space of school geometry, as distance is synonymous with similarity. How close (similar) or far away are two points? Can we group them together? With Euclid's help, we can approach unsupervised learning with k-means clustering and place points in categories we do not know in advance.

Chapter 7, *Cross-Validation and Post-Model Workflow*, features how to select a model that works well with cross-validation: iterated training and testing of predictions. We also save computational work with the pickle module.

Chapter 8, *Support Vector Machines*, examines in detail the support vector machine, a powerful and easy-to-understand algorithm.

Chapter 9, *Tree Algorithms and Ensembles*, features the algorithms of decision making: decision trees. This chapter introduces meta-learning algorithms, diverse algorithms that vote in some fashion to increase overall predictive accuracy.

Chapter 10, *Text and Multiclass Classification with scikit-learn*, reviews the basics of natural language processing with the simple bag-of-words model. In general, we view classification with three or more categories.

Chapter 11, *Neural Networks*, introduces a neural network and perceptrons, the components of a neural network. Each layer figures out a step in a process, leading to a desired outcome. As we do not program any steps specifically, we venture into artificial intelligence. Save the neural network so that you can keep training it later, or load it and utilize it as part of a stacking ensemble.

Chapter 12, *Create a Simple Estimator*, helps you make your own scikit-learn estimator, which you can contribute to the scikit-learn community and take part in the evolution of data science with scikit-learn.

Who this book is for

This book is for data analysts who are familiar with Python but not so much with scikit-learn, and Python programmers who would like to dive into the world of machine learning in a direct, straightforward fashion.

What you need for this book

You will need to install following libraries:

- anaconda 4.1.1
- numba 0.26.0
- numpy 1.12.1
- pandas 0.20.3
- pandas-datareader 0.4.0
- patsy 0.4.1
- scikit-learn 0.19.0
- scipy 0.19.1
- statsmodels 0.8.0
- sympy 1.0

Conventions

In this book, you will find a number of text styles that distinguish between different kinds of information. Here are some examples of these styles and an explanation of their meaning.

Code words in text, database table names, folder names, filenames, file extensions, pathnames, dummy URLs, user input, and Twitter handles are shown as follows: "The `scikit-learn` library requires input tables of two-dimensional NumPy arrays."

Any command-line input or output is written as follows:

```
import numpy as np #Load the numpy library for fast array
computations
import pandas as pd #Load the pandas data-analysis library
import matplotlib.pyplot as plt #Load the pyplot visualization
library
```

New terms and **important words** are shown in bold.



Warnings or important notes appear in a box like this.



Tips and tricks appear like this.

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1

High-Performance Machine Learning – NumPy

In this chapter, we will cover the following recipes:

- NumPy basics
- Loading the iris dataset
- Viewing the iris dataset
- Viewing the iris dataset with pandas
- Plotting with NumPy and matplotlib
- A minimal machine learning recipe – SVM classification
- Introducing cross-validation
- Putting it all together
- Machine learning overview – classification versus regression

Introduction

In this chapter, we'll learn how to make predictions with scikit-learn. Machine learning emphasizes on measuring the ability to predict, and with scikit-learn we will predict accurately and quickly.

We will examine the `iris` dataset, which consists of measurements of three types of Iris flowers: *Iris Setosa*, *Iris Versicolor*, and *Iris Virginica*.

To measure the strength of the predictions, we will:

- Save some data for testing
- Build a model using only training data
- Measure the predictive power on the test set

The prediction—one of three flower types is categorical. This type of problem is called a **classification problem**.

Informally, classification asks, *Is it an apple or an orange?* Contrast this with machine learning regression, which asks, *How many apples?* By the way, the answer can be *4.5 apples* for regression.

By the evolution of its design, scikit-learn addresses machine learning mainly via four categories:

- Classification:
 - Non-text classification, like the Iris flowers example
 - Text classification
- Regression
- Clustering
- Dimensionality reduction

NumPy basics

Data science deals in part with structured tables of data. The `scikit-learn` library requires input tables of two-dimensional NumPy arrays. In this section, you will learn about the `numpy` library.

How to do it...

We will try a few operations on NumPy arrays. NumPy arrays have a single type for all of their elements and a predefined shape. Let us look first at their shape.

The shape and dimension of NumPy arrays

1. Start by importing NumPy:

```
import numpy as np
```

2. Produce a NumPy array of 10 digits, similar to Python's `range(10)` method:

```
np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

3. The array looks like a Python list with only one pair of brackets. This means it is of one dimension. Store the array and find out the shape:

```
array_1 = np.arange(10)
array_1.shape
(10L,)
```

4. The array has a data attribute, `shape`. The type of `array_1.shape` is a tuple `(10L,)`, which has length 1, in this case. The number of dimensions is the same as the length of the tuple—a dimension of 1, in this case:

```
array_1.ndim      #Find number of dimensions of array_1
1
```

5. The array has 10 elements. Reshape the array by calling the `reshape` method:

```
array_1.reshape((5,2))
array([[0, 1],
       [2, 3],
       [4, 5],
       [6, 7],
       [8, 9]])
```

6. This reshapes the array into 5×2 data object that resembles a list of lists (a three dimensional NumPy array looks like a list of lists of lists). You did not save the changes. Save the reshaped array as follows::

```
array_1 = array_1.reshape((5,2))
```

7. Note that `array_1` is now two-dimensional. This is expected, as its shape has two numbers and it looks like a Python list of lists:

```
array_1.ndim  
2
```

NumPy broadcasting

8. Add 1 to every element of the array by broadcasting. Note that changes to the array are not saved:

```
array_1 + 1  
array([[ 1,  2],  
       [ 3,  4],  
       [ 5,  6],  
       [ 7,  8],  
       [ 9, 10]])
```

The term **broadcasting** refers to the smaller array being stretched or broadcast across the larger array. In the first example, the scalar 1 was stretched to a 5 x 2 shape and then added to `array_1`.

9. Create a new `array_2` array. Observe what occurs when you multiply the array by itself (this is not matrix multiplication; it is element-wise multiplication of arrays):

```
array_2 = np.arange(10)  
array_2 * array_2  
array([ 0,  1,  4,  9, 16, 25, 36, 49, 64, 81])
```

10. Every element has been squared. Here, element-wise multiplication has occurred. Here is a more complicated example:

```
array_2 = array_2 ** 2 #Note that this is equivalent to array_2 *  
array_2  
array_2 = array_2.reshape((5,2))  
array_2  
array([[ 0,  1],  
       [ 4,  9],  
       [16, 25],  
       [36, 49],  
       [64, 81]])
```

11. Change `array_1` as well:

```
array_1 = array_1 + 1
array_1
array([[ 1,  2],
       [ 3,  4],
       [ 5,  6],
       [ 7,  8],
       [ 9, 10]])
```

12. Now add `array_1` and `array_2` element-wise by simply placing a plus sign between the arrays:

```
array_1 + array_2
array([[ 1,  3],
       [ 7, 13],
       [21, 31],
       [43, 57],
       [73, 91]])
```

13. The formal broadcasting rules require that whenever you are comparing the shapes of both arrays from right to left, all the numbers have to either match or be one. The shapes `5 X 2` and `5 X 2` match for both entries from right to left. However, the shape `5 X 2 X 1` does not match `5 X 2`, as the second values from the right, `2` and `5` respectively, are mismatched:

Shape Match	Shape Mismatch
5 X 2	5 X 2 X 1
5 X 2	5 X 2
Shape Match	Shape Match
5 X 1	5 X 2 X 5
1 X 5	1 X 2 X 5
Shape Match	Shape Mismatch
1 X 2	1 X 5 X 2
2 X 1	1 X 2 X 5

Initializing NumPy arrays and dtypes

There are several ways to initialize NumPy arrays besides `np.arange`:

14. Initialize an array of zeros with `np.zeros`. The `np.zeros((5,2))` command creates a 5 x 2 array of zeros:

```
np.zeros((5,2))
array([[ 0.,  0.],
       [ 0.,  0.],
       [ 0.,  0.],
       [ 0.,  0.],
       [ 0.,  0.]])
```

15. Initialize an array of ones using `np.ones`. Introduce a `dtype` argument, set to `np.int`, to ensure that the ones are of NumPy integer type. Note that scikit-learn expects `np.float` arguments in arrays. The `dtype` refers to the type of every element in a NumPy array. It remains the same throughout the array. Every single element of the array below has a `np.int` integer type.

```
np.ones((5,2), dtype = np.int)
array([[1, 1],
       [1, 1],
       [1, 1],
       [1, 1],
       [1, 1]])
```

16. Use `np.empty` to allocate memory for an array of a specific size and `dtype`, but no particular initialized values:

```
np.empty((5,2), dtype = np.float)
array([[ 3.14724935e-316,  3.14859499e-316],
       [ 3.14858945e-316,  3.14861159e-316],
       [ 3.14861435e-316,  3.14861712e-316],
       [ 3.14861989e-316,  3.14862265e-316],
       [ 3.14862542e-316,  3.14862819e-316]])
```

17. Use `np.zeros`, `np.ones`, and `np.empty` to allocate memory for NumPy arrays with different initial values.

Indexing

18. Look up the values of the two-dimensional arrays with indexing:

```
array_1[0,0]    #Finds value in first row and first column.  
1
```

19. View the first row:

```
array_1[0, :]  
array([1, 2])
```

20. Then view the first column:

```
array_1[:, 0]  
array([1, 3, 5, 7, 9])
```

21. View specific values along both axes. Also view the second to the fourth rows:

```
array_1[2:5, :]  
array([[ 5,  6],  
       [ 7,  8],  
       [ 9, 10]])
```

22. View the second to the fourth rows only along the first column:

```
array_1[2:5, 0]  
array([5, 7, 9])
```

Boolean arrays

Additionally, NumPy handles indexing with Boolean logic:

23. First produce a Boolean array:

```
array_1 > 5  
array([[False, False],  
       [False, False],  
       [False, True],  
       [ True,  True],  
       [ True,  True]], dtype=bool)
```

24. Place brackets around the Boolean array to filter by the Boolean array:

```
array_1[array_1 > 5]
array([ 6,  7,  8,  9, 10])
```

Arithmetic operations

25. Add all the elements of the array with the `sum` method. Go back to `array_1`:

```
array_1
array([[ 1,  2],
       [ 3,  4],
       [ 5,  6],
       [ 7,  8],
       [ 9, 10]])
array_1.sum()
55
```

26. Find all the sums by row:

```
array_1.sum(axis = 1)
array([ 3,  7, 11, 15, 19])
```

27. Find all the sums by column:

```
array_1.sum(axis = 0)
array([25, 30])
```

28. Find the mean of each column in a similar way. Note that the `dtype` of the array of averages is `np.float`:

```
array_1.mean(axis = 0)
array([ 5.,  6.])
```

NaN values

29. Scikit-learn will not accept `np.nan` values. Take `array_3` as follows:

```
array_3 = np.array([np.nan, 0, 1, 2, np.nan])
```

30. Find the NaN values with a special Boolean array created by the `np.isnan` function:

```
np.isnan(array_3)
array([ True, False, False, False,  True], dtype=bool)
```

31. Filter the NaN values by negating the Boolean array with the symbol `~` and placing brackets around the expression:

```
array_3[~np.isnan(array_3)]
>array([ 0.,  1.,  2.])
```

32. Alternatively, set the NaN values to zero:

```
array_3[np.isnan(array_3)] = 0
array_3
array([ 0.,  0.,  1.,  2.,  0.])
```

How it works...

Data, in the present and minimal sense, is about 2D tables of numbers, which NumPy handles very well. Keep this in mind in case you forget the NumPy syntax specifics. Scikit-learn accepts only 2D NumPy arrays of real numbers with no missing `np.nan` values.

From experience, it tends to be best to change `np.nan` to some value instead of throwing away data. Personally, I like to keep track of Boolean masks and keep the data shape roughly the same, as this leads to fewer coding errors and more coding flexibility.

Loading the iris dataset

To perform machine learning with scikit-learn, we need some data to start with. We will load the `iris` dataset, one of the several datasets available in scikit-learn.

Getting ready

A scikit-learn program begins with several imports. Within Python, preferably in Jupyter Notebook, load the `numpy`, `pandas`, and `pyplot` libraries:

```
import numpy as np      #Load the numpy library for fast array
                           computations
import pandas as pd     #Load the pandas data-analysis library
import matplotlib.pyplot as plt  #Load the pyplot visualization
                           library
```

If you are within a Jupyter Notebook, type the following to see a graphical output instantly:

```
%matplotlib inline
```

How to do it...

1. From the scikit-learn `datasets` module, access the `iris` dataset:

```
from sklearn import datasets
iris = datasets.load_iris()
```

How it works...

Similarly, you could have imported the `diabetes` dataset as follows:

```
from sklearn import datasets  #Import datasets module from scikit-learn
diabetes = datasets.load_diabetes()
```

There! You've loaded `diabetes` using the `load_diabetes()` function of the `datasets` module. To check which datasets are available, type:

```
datasets.load_*
```

Once you try that, you might observe that there is a dataset named `datasets.load_digits`. To access it, type the `load_digits()` function, analogous to the other loading functions:

```
digits = datasets.load_digits()
```

To view information about the dataset, type `digits.DESCR`.

Viewing the iris dataset

Now that we've loaded the dataset, let's examine what is in it. The `iris` dataset pertains to a supervised classification problem.

How to do it...

1. To access the observation variables, type:

```
iris.data
```

This outputs a NumPy array:

```
array([[ 5.1,  3.5,  1.4,  0.2],
       [ 4.9,  3. ,  1.4,  0.2],
       [ 4.7,  3.2,  1.3,  0.2],
       #...rest of output suppressed because of length
```

2. Let's examine the NumPy array:

```
iris.data.shape
```

This returns:

```
(150L, 4L)
```

This means that the data is 150 rows by 4 columns. Let's look at the first row:

```
iris.data[0]
array([ 5.1,  3.5,  1.4,  0.2])
```

The NumPy array for the first row has four numbers.

3. To determine what they mean, type:

```
iris.feature_names
['sepal length (cm)',
 'sepal width (cm)',
 'petal length (cm)',
 'petal width (cm)']
```

The feature or column names name the data. They are strings, and in this case, they correspond to dimensions in different types of flowers. Putting it all together, we have 150 examples of flowers with four measurements per flower in centimeters. For example, the first flower has measurements of 5.1 cm for sepal length, 3.5 cm for sepal width, 1.4 cm for petal length, and 0.2 cm for petal width. Now, let's look at the output variable in a similar manner:

```
iris.target
```

This yields an array of outputs: 0, 1, and 2. There are only three outputs. Type this:

```
iris.target.shape
```

You get a shape of:

```
(150L,)
```

This refers to an array of length 150 (150 x 1). Let's look at what the numbers refer to:

```
iris.target_names
```

```
array(['setosa', 'versicolor', 'virginica'],  
      dtype='<S10')
```

The output of the `iris.target_names` variable gives the English names for the numbers in the `iris.target` variable. The number zero corresponds to the `setosa` flower, number one corresponds to the `versicolor` flower, and number two corresponds to the `virginica` flower. Look at the first row of `iris.target`:

```
iris.target[0]
```

This produces zero, and thus the first row of observations we examined before correspond to the `setosa` flower.

How it works...

In machine learning, we often deal with data tables and two-dimensional arrays corresponding to examples. In the `iris` set, we have 150 observations of flowers of three types. With new observations, we would like to predict which type of flower those observations correspond to. The observations in this case are measurements in centimeters. It is important to look at the data pertaining to real objects. Quoting my high school physics teacher, *"Do not forget the units!"*

The `iris` dataset is intended to be for a supervised machine learning task because it has a target array, which is the variable we desire to predict from the observation variables. Additionally, it is a classification problem, as there are three numbers we can predict from the observations, one for each type of flower. In a classification problem, we are trying to distinguish between categories. The simplest case is binary classification. The `iris` dataset, with three flower categories, is a multi-class classification problem.

There's more...

With the same data, we can rephrase the problem in many ways, or formulate new problems. What if we want to determine relationships between the observations? We can define the petal width as the target variable. We can rephrase the problem as a regression problem and try to predict the target variable as a real number, not just three categories. Fundamentally, it comes down to what we intend to predict. Here, we desire to predict a type of flower.

Viewing the iris dataset with Pandas

In this recipe we will use the handy `pandas` data analysis library to view and visualize the `iris` dataset. It contains the notion of a dataframe which might be familiar to you if you use the language R's dataframe.

How to do it...

You can view the `iris` dataset with Pandas, a library built on top of NumPy:

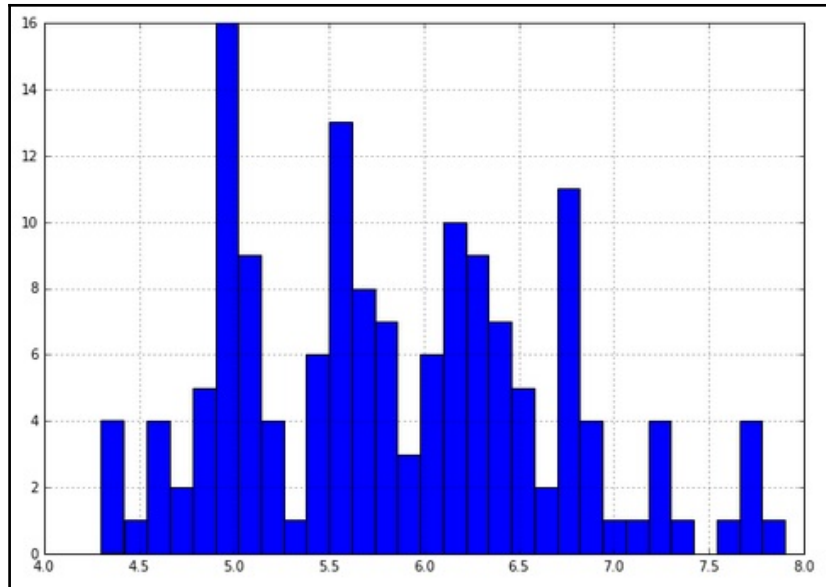
1. Create a dataframe with the observation variables `iris.data`, and column names `columns`, as arguments:

```
import pandas as pd
iris_df = pd.DataFrame(iris.data, columns = iris.feature_names)
```

The dataframe is more user-friendly than the NumPy array.

2. Look at a quick histogram of the values in the dataframe for `sepal length`:

```
iris_df['sepal length (cm)'].hist(bins=30)
```



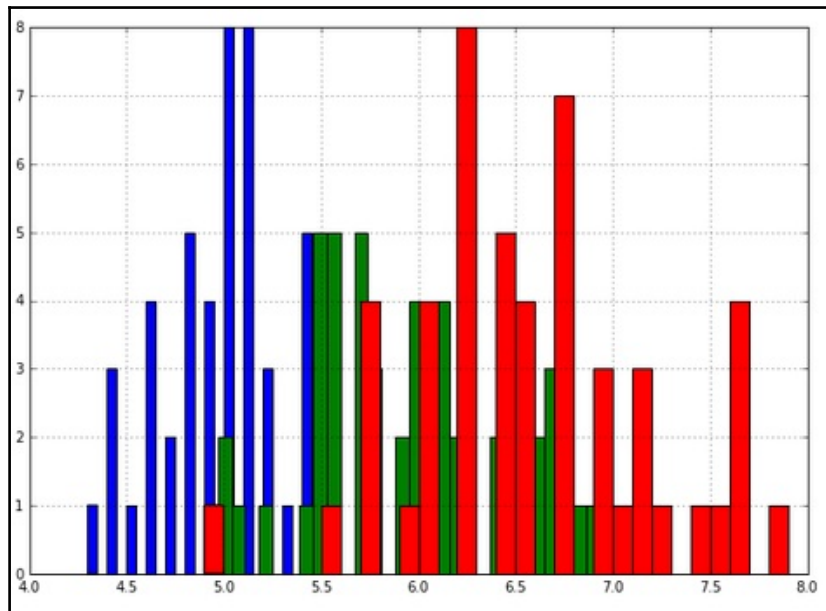
3. You can also color the histogram by the `target` variable:

```
for class_number in np.unique(iris.target):  
    plt.figure(1)  
    iris_df['sepal length (cm)'].iloc[np.where(iris.target ==  
class_number)[0]].hist(bins=30)
```

4. Here, iterate through the target numbers for each flower and draw a color histogram for each. Consider this line:

```
np.where(iris.target== class_number)[0]
```


It finds the NumPy index location for each class of flower:



Observe that the histograms overlap. This encourages us to model the three histograms as three normal distributions. This is possible in a machine learning manner if we model the training data only as three normal distributions, not the whole set. Then we use the test set to test the three normal distribution models we just made up. Finally, we test the accuracy of our predictions on the test set.

How it works...

The dataframe data object is a 2D NumPy array with column names and row names. In data science, the fundamental data object looks like a 2D table, possibly because of SQL's long history. NumPy allows for 3D arrays, cubes, 4D arrays, and so on. These also come up often.

Plotting with NumPy and matplotlib

A simple way to make visualizations with NumPy is by using the library `matplotlib`. Let's make some visualizations quickly.

Getting ready

Start by importing `numpy` and `matplotlib`. You can view visualizations within an IPython Notebook using the `%matplotlib inline` command:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

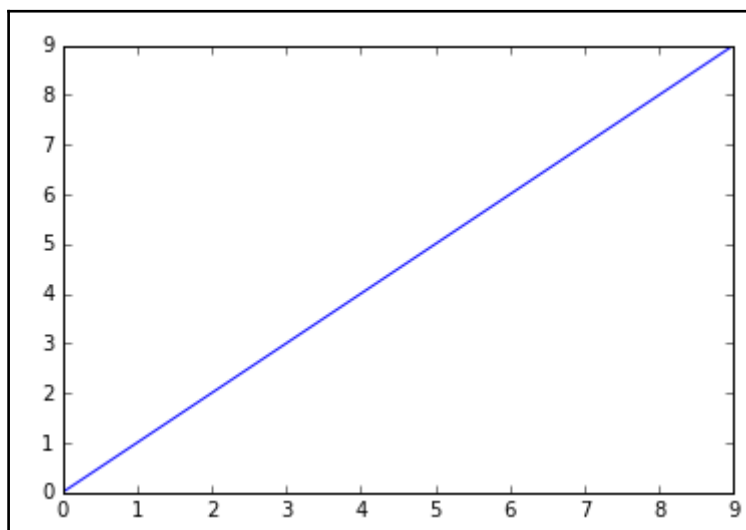
How to do it...

1. The main command in `matplotlib`, in pseudo code, is as follows:

```
plt.plot(numpy array, numpy array of same length)
```

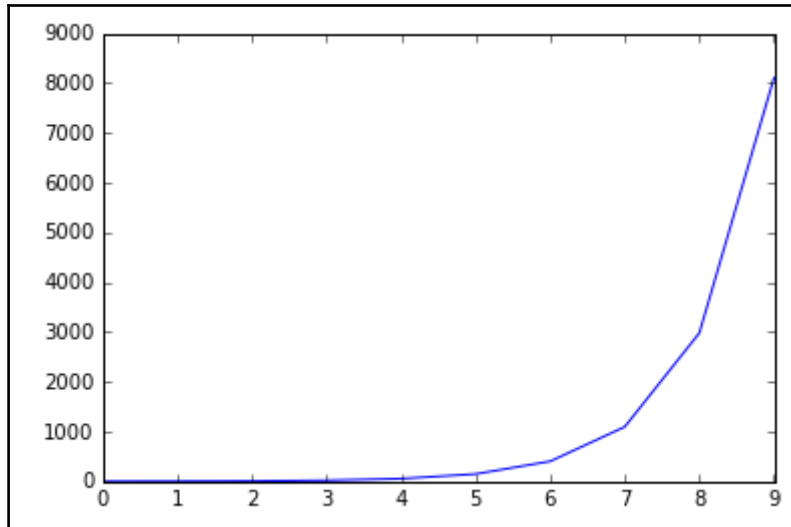
2. Plot a straight line by placing two NumPy arrays of the same length:

```
plt.plot(np.arange(10), np.arange(10))
```



3. Plot an exponential:

```
plt.plot(np.arange(10), np.exp(np.arange(10)))
```

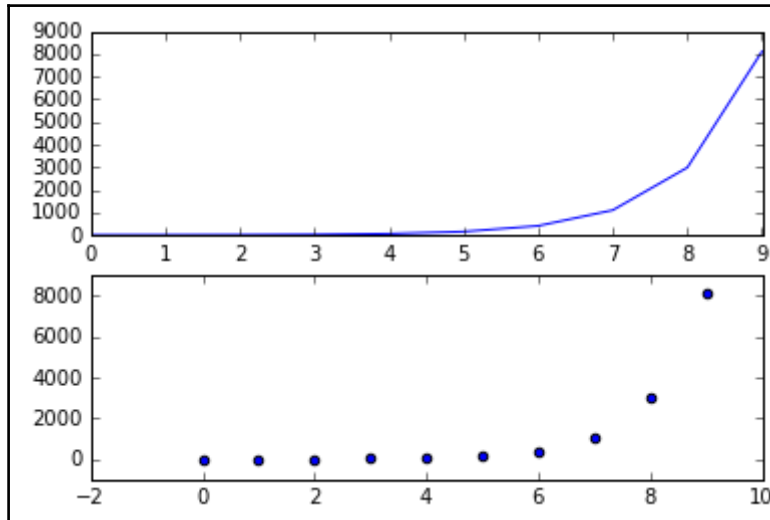


4. Place the two graphs side by side:

```
plt.figure()  
plt.subplot(121)  
plt.plot(np.arange(10), np.exp(np.arange(10)))  
plt.subplot(122)  
plt.scatter(np.arange(10), np.exp(np.arange(10)))
```

Or top to bottom:

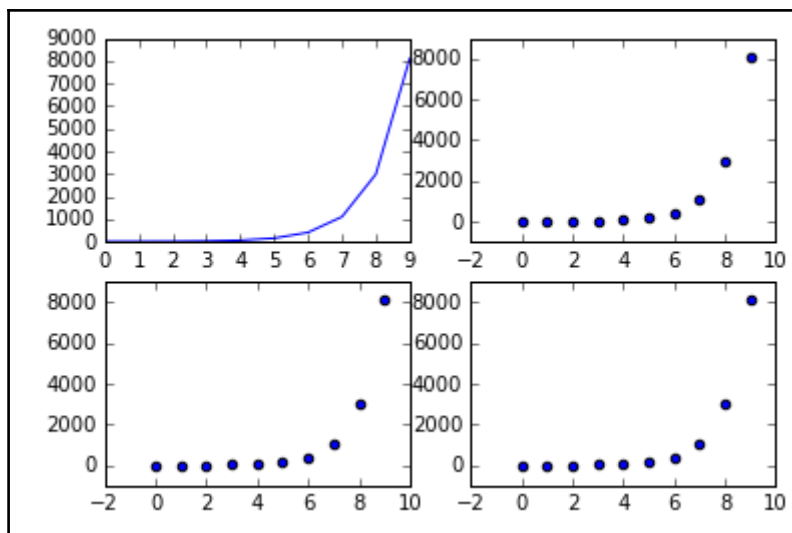
```
plt.figure()
plt.subplot(211)
plt.plot(np.arange(10), np.exp(np.arange(10)))
plt.subplot(212)
plt.scatter(np.arange(10), np.exp(np.arange(10)))
```



The first two numbers in the subplot command refer to the grid size in the figure instantiated by `plt.figure()`. The grid size referred to in `plt.subplot(221)` is 2×2 , the first two digits. The last digit refers to traversing the grid in reading order: left to right and then up to down.

5. Plot in a 2×2 grid traversing in reading order from one to four:

```
plt.figure()
plt.subplot(221)
plt.plot(np.arange(10), np.exp(np.arange(10)))
plt.subplot(222)
plt.scatter(np.arange(10), np.exp(np.arange(10)))
plt.subplot(223)
plt.scatter(np.arange(10), np.exp(np.arange(10)))
plt.subplot(224)
plt.scatter(np.arange(10), np.exp(np.arange(10)))
```



6. Finally, with real data:

```
from sklearn.datasets import load_iris

iris = load_iris()
data = iris.data
target = iris.target

# Resize the figure for better viewing
plt.figure(figsize=(12,5))

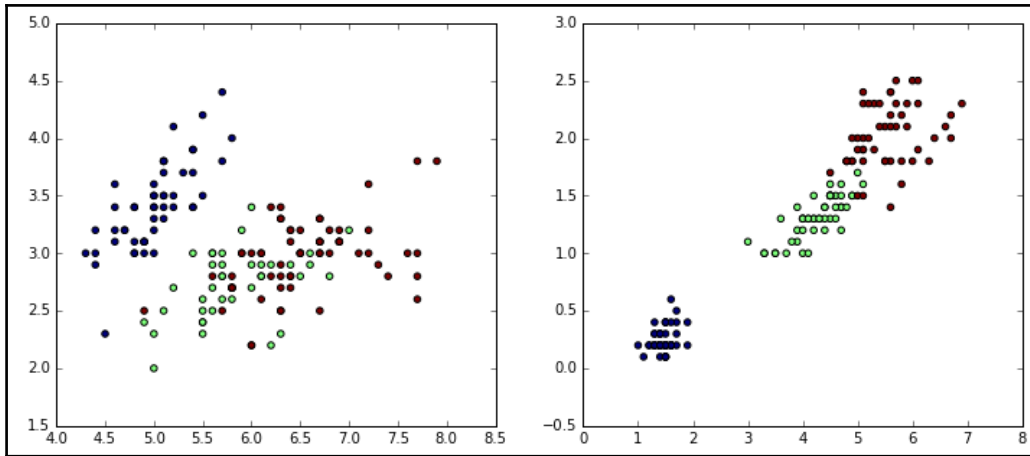
# First subplot
plt.subplot(121)

# Visualize the first two columns of data:
plt.scatter(data[:,0], data[:,1], c=target)

# Second subplot
plt.subplot(122)

# Visualize the last two columns of data:
plt.scatter(data[:,2], data[:,3], c=target)
```

The `c` parameter takes an array of colors—in this case, the colors 0, 1, and 2 in the `iris` target:



A minimal machine learning recipe – SVM classification

Machine learning is all about making predictions. To make predictions, we will:

- State the problem to be solved
- Choose a model to solve the problem
- Train the model
- Make predictions
- Measure how well the model performed

Getting ready

Back to the `iris` example, we now store the first two features (columns) of the observations as `x` and the target as `y`, a convention in the machine learning community:

```
x = iris.data[:, :2]
y = iris.target
```

How to do it...

1. First, we state the problem. We are trying to determine the flower-type category from a set of new observations. This is a classification task. The data available includes a target variable, which we have named y . This is a supervised classification problem.



The task of supervised learning involves predicting values of an output variable with a model that trains using input variables and an output variable.

2. Next, we choose a model to solve the supervised classification. For now, we will use a support vector classifier. Because of its simplicity and interpretability, it is a commonly used algorithm (*interpretable* means easy to read into and understand).
3. To measure the performance of prediction, we will split the dataset into training and test sets. The training set refers to data we will learn from. The test set is the data we hold out and pretend not to know as we would like to measure the performance of our learning procedure. So, import a function that will split the dataset:

```
from sklearn.model_selection import train_test_split
```

4. Apply the function to both the observation and target data:

```
X_train, X_test, y_train, y_test = train_test_split(X, y,  
test_size=0.25, random_state=1)
```

The test size is 0.25 or 25% of the whole dataset. A random state of one fixes the random seed of the function so that you get the same results every time you call the function, which is important for now to reproduce the same results consistently.

5. Now load a regularly used estimator, a support vector machine:

```
from sklearn.svm import SVC
```

6. You have imported a support vector classifier from the `svm` module. Now create an instance of a linear SVC:

```
clf = SVC(kernel='linear', random_state=1)
```

The random state is fixed to reproduce the same results with the same code later.

The supervised models in scikit-learn implement a `fit(X, y)` method, which trains the model and returns the trained model. `x` is a subset of the observations, and each element of `y` corresponds to the target of each observation in `x`. Here, we fit a model on the training data:

```
clf.fit(X_train, y_train)
```

Now, the `clf` variable is the fitted, or trained, model.

The estimator also has a `predict(X)` method that returns predictions for several unlabeled observations, `X_test`, and returns the predicted values, `y_pred`. Note that the function does not return the estimator. It returns a set of predictions:

```
y_pred = clf.predict(X_test)
```

So far, you have done all but the last step. To examine the model performance, load a scorer from the metrics module:

```
from sklearn.metrics import accuracy_score
```

With the scorer, compare the predictions with the held-out test targets:

```
accuracy_score(y_test, y_pred)
```

```
0.76315789473684215
```

How it works...

Without knowing very much about the details of support vector machines, we have implemented a predictive model. To perform machine learning, we held out one-fourth of the data and examined how the SVC performed on that data. In the end, we obtained a number that measures accuracy, or how the model performed.

There's more...

To summarize, we will do all the steps with a different algorithm, logistic regression:

1. First, import `LogisticRegression`:

```
from sklearn.linear_model import LogisticRegression
```


2. Then write a program with the modeling steps:
 1. Split the data into training and testing sets.
 2. Fit the logistic regression model.
 3. Predict using the test observations.
 4. Measure the accuracy of the predictions with `y_test` versus `y_pred`:

```
import matplotlib.pyplot as plt
from sklearn import datasets

from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

X = iris.data[:, :2]    #load the iris data
y = iris.target
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25,
random_state=1)

#train the model
clf = LogisticRegression(random_state = 1)
clf.fit(X_train, y_train)

#predict with Logistic Regression
y_pred = clf.predict(X_test)

#examine the model accuracy
accuracy_score(y_test, y_pred)

0.60526315789473684
```

This number is lower; yet we cannot make any conclusions comparing the two models, SVC and logistic regression classification. We cannot compare them, because we were not supposed to look at the test set for our model. If we made a choice between SVC and logistic regression, the choice would be part of our model as well, so the test set cannot be involved in the choice. Cross-validation, which we will look at next, is a way to choose between models.

Introducing cross-validation

We are thankful for the `iris` dataset, but as you might recall, it has only 150 observations. To make the most out of the set, we will employ cross-validation. Additionally, in the last section, we wanted to compare the performance of two different classifiers, support vector classifier and logistic regression. Cross-validation will help us with this comparison issue as well.

Getting ready

Suppose we wanted to choose between the support vector classifier and the logistic regression classifier. We cannot measure their performance on the unavailable test set.

What if, instead, we:

- Forgot about the test set for now?
- Split the training set into two parts, one to train on and one to test the training?

Split the training set into two parts using the `train_test_split` function used in previous sections:

```
from sklearn.model_selection import train_test_split
X_train_2, X_test_2, y_train_2, y_test_2 = train_test_split(X_train,
y_train, test_size=0.25, random_state=1)
```

`X_train_2` consists of 75% of the `X_train` data, while `X_test_2` is the remaining 25%. `y_train_2` is 75% of the target data, and matches the observations of `X_train_2`. `y_test_2` is 25% of the target data present in `y_train`.

As you might have expected, you have to use these new splits to choose between the two models: SVC and logistic regression. Do so by writing a predictive program.

How to do it...

1. Start with all the imports and load the `iris` dataset:

```
from sklearn import datasets

from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

#load the classifying models
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC

iris = datasets.load_iris()
X = iris.data[:, :2] #load the first two features of the iris data
y = iris.target #load the target of the iris data

#split the whole set one time
#Note random state is 7 now
X_train, X_test, y_train, y_test = train_test_split(X, y,
```

```
test_size=0.25, random_state=7)

#split the training set into parts
X_train_2, X_test_2, y_train_2, y_test_2 =
train_test_split(X_train, y_train, test_size=0.25, random_state=7)
```

2. Create an instance of an SVC classifier and fit it:

```
svc_clf = SVC(kernel = 'linear', random_state = 7)
svc_clf.fit(X_train_2, y_train_2)
```

3. Do the same for logistic regression (both lines for logistic regression are compressed into one):

```
lr_clf = LogisticRegression(random_state = 7).fit(X_train_2,
y_train_2)
```

4. Now predict and examine the SVC and logistic regression's performance on X_test_2:

```
svc_pred = svc_clf.predict(X_test_2)
lr_pred = lr_clf.predict(X_test_2)

print "Accuracy of SVC:", accuracy_score(y_test_2, svc_pred)
print "Accuracy of LR:", accuracy_score(y_test_2, lr_pred)

Accuracy of SVC: 0.857142857143
Accuracy of LR: 0.714285714286
```

5. The SVC performs better, but we have not yet seen the original test data. Choose SVC over logistic regression and try it on the original test set:

```
print "Accuracy of SVC on original Test Set:
", accuracy_score(y_test, svc_clf.predict(X_test))

Accuracy of SVC on original Test Set: 0.684210526316
```

How it works...

In comparing the SVC and logistic regression classifier, you might wonder (and be a little suspicious) about a lot of scores being very different. The final test on SVC scored lower than logistic regression. To help with this situation, we can do cross-validation in scikit-learn.

Cross-validation involves splitting the training set into parts, as we did before. To match the preceding example, we split the training set into four parts, or folds. We are going to design a cross-validation iteration by taking turns with one of the four folds for testing and the other three for training. It is the same split as done before four times over with the same set, thereby rotating, in a sense, the test set:

All Data	Fold 1	Fold 2	Fold 3	Fold 4
CV Set	Test	Train	Train	Train
	Train	Test	Train	Train
	Train	Train	Test	Train
	Train	Train	Train	Test
Final Test	Final Test	Final Test	Final Test	Final Test

With scikit-learn, this is relatively easy to accomplish:

1. We start with an import:

```
from sklearn.model_selection import cross_val_score
```

2. Then we produce an accuracy score on four folds:

```
svc_scores = cross_val_score(svc_clf, X_train, y_train, cv=4)
svc_scores
```

```
array([ 0.82758621,  0.85714286,  0.92857143,  0.77777778])
```

3. We can find the mean for average performance and standard deviation for a measure of spread of all scores relative to the mean:

```
print "Average SVC scores: ", svc_scores.mean()
print "Standard Deviation of SVC scores: ", svc_scores.std()
```

```
Average SVC scores:  0.847769567597
Standard Deviation of SVC scores:  0.0545962864696
```

4. Similarly, with the logistic regression instance, we compute four scores:

```
lr_scores = cross_val_score(lr_clf, X_train, y_train, cv=4)
print "Average SVC scores: ", lr_scores.mean()
print "Standard Deviation of SVC scores: ", lr_scores.std()
```

```
Average SVC scores:  0.748893906221
Standard Deviation of SVC scores:  0.0485633168699
```

Now we have many scores, which confirms our selection of SVC over logistic regression. Thanks to cross-validation, we used the training multiple times and had four small test sets within it to score our model.

Note that our model is a bigger model that consists of:

- Training an SVM through cross-validation
- Training a logistic regression through cross-validation
- Choosing between SVM and logistic regression



The choice at the end is part of the model.

There's more...

Despite our hard work and the elegance of the scikit-learn syntax, the score on the test set at the very end remains suspicious. The reason for this is that the test and train split are not necessarily balanced; the train and test sets do not necessarily have similar proportions of all the classes.

This is easily remedied by using a stratified test-train split:

```
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y)
```

By selecting the target set as the stratified argument, the target classes are balanced. This brings the SVC scores closer together.

```
svc_scores = cross_val_score(svc_clf, X_train, y_train, cv=4)
print "Average SVC scores: " , svc_scores.mean()
print "Standard Deviation of SVC scores: ", svc_scores.std()
print "Score on Final Test Set:", accuracy_score(y_test,
svc_clf.predict(X_test))
```

```
Average SVC scores:  0.831547619048
Standard Deviation of SVC scores:  0.0792488953372
Score on Final Test Set: 0.789473684211
```

Additionally, note that in the preceding example, the cross-validation procedure produces stratified folds by default:

```
from sklearn.model_selection import cross_val_score
svc_scores = cross_val_score(svc_clf, X_train, y_train, cv = 4)
```

The preceding code is equivalent to:

```
from sklearn.model_selection import cross_val_score, StratifiedKfold
skf = StratifiedKfold(n_splits = 4)
svc_scores = cross_val_score(svc_clf, X_train, y_train, cv = skf)
```

Putting it all together

Now, we are going to perform the same procedure as before, except that we will reset, regroup, and try a new algorithm: **K-Nearest Neighbors (KNN)**.

How to do it...

1. Start by importing the model from `sklearn`, followed by a balanced split:

```
from sklearn.neighbors import KNeighborsClassifier
X_train, X_test, y_train, y_test = train_test_split(X, y,
stratify=y, random_state = 0)
```



The `random_state` parameter fixes the `random_seed` in the function `train_test_split`. In the preceding example, the `random_state` is set to zero and can be set to any integer.

2. Construct two different KNN models by varying the `n_neighbors` parameter. Observe that the number of folds is now 10. Tenfold cross-validation is common in the machine learning community, particularly in data science competitions:

```
from sklearn.model_selection import cross_val_score
knn_3_clf = KNeighborsClassifier(n_neighbors = 3)
knn_5_clf = KNeighborsClassifier(n_neighbors = 5)

knn_3_scores = cross_val_score(knn_3_clf, X_train, y_train, cv=10)
knn_5_scores = cross_val_score(knn_5_clf, X_train, y_train, cv=10)
```

3. Score and print out the scores for selection:

```
print "knn_3 mean scores: ", knn_3_scores.mean(), "knn_3 std: ", knn_3_scores.std()
print "knn_5 mean scores: ", knn_5_scores.mean(), "knn_5 std: ", knn_5_scores.std()

knn_3 mean scores:  0.798333333333 knn_3 std:  0.0908142181722
knn_5 mean scores:  0.806666666667 knn_5 std:  0.0559320575496
```

Both nearest neighbor types score similarly, yet the KNN with parameter `n_neighbors = 5` is a bit more stable. This is an example of *hyperparameter optimization* which we will examine closely throughout the book.

There's more...

You could have just as easily run a simple loop to score the function more quickly:

```
all_scores = []
for n_neighbors in range(3,9,1):
    knn_clf = KNeighborsClassifier(n_neighbors = n_neighbors)
    all_scores.append((n_neighbors, cross_val_score(knn_clf, X_train,
y_train, cv=10).mean()))
sorted(all_scores, key = lambda x:x[1], reverse = True)
```

Its output suggests that `n_neighbors = 4` is a good choice:

```
[(4, 0.8511111111111115),
 (7, 0.8261111111111113),
 (6, 0.8233333333333334),
 (5, 0.8066666666666664),
 (3, 0.7983333333333334),
 (8, 0.7983333333333334)]
```

Machine learning overview – classification versus regression

In this recipe we will examine how regression can be viewed as being very similar to classification. This is done by reconsidering the categorical labels of regression as real numbers. In this section we will also look at several aspects of machine learning from a very broad perspective including the purpose of scikit-learn. scikit-learn allows us to find models that work well incredibly quickly. We do not have to work out all the details of the model, or optimize, until we found one that works well. Consequently, your company saves precious development time and computational resources thanks to scikit-learn giving us the ability to develop models relatively quickly.

The purpose of scikit-learn

As we have seen before, scikit-learn allowed us to find a model that works fairly quickly. We tried SVC, logistic regression, and a few KNN classifiers. Through cross-validation, we selected models that performed better than others. In industry, after trying SVMs and logistic regression, we might focus on SVMs and optimize them further. Thanks to scikit-learn, we saved a lot of time and resources, including mental energy. After optimizing the SVM at work on a realistic dataset, we might re-implement it for speed in Java or C and gather more data.

Supervised versus unsupervised

Classification and regression are supervised, as we know the target variables for the observations. Clustering—creating regions in space for each category without being given any labels is unsupervised learning.

Getting ready

In classification, the target variable is one of several categories, and there must be more than one instance of every category. In regression, there can be only one instance of every target variable, as the only requirement is that the target is a real number.

In the case of logistic regression, we saw previously that the algorithm first performs a regression and estimates a real number for the target. Then the target class is estimated by using thresholds. In scikit-learn, there are `predict_proba` methods that yield probabilistic estimates, which relate regression-like real number estimates with classification classes in the style of logistic regression.

Any regression can be turned into classification by using thresholds. A binary classification can be viewed as a regression problem by using a regressor. The target variables produced will be real numbers, not the original class variables.

How to do it...

Quick SVC – a classifier and regressor

1. Load `iris` from the `datasets` module:

```
import numpy as np
import pandas as pd
from sklearn import datasets

iris = datasets.load_iris()
```

2. For simplicity, consider only targets 0 and 1, corresponding to Setosa and Versicolor. Use the Boolean array `iris.target < 2` to filter out target 2. Place it within brackets to use it as a filter in defining the observation set `x` and the target set `y`:

```
x = iris.data[iris.target < 2]
y = iris.target[iris.target < 2]
```

3. Now import `train_test_split` and apply it:

```
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    stratify=y, random_state= 7)
```

4. Prepare and run an SVC by importing it and scoring it with cross-validation:

```
from sklearn.svm import SVC
from sklearn.model_selection import cross_val_score

svc_clf = SVC(kernel = 'linear').fit(X_train, y_train)
svc_scores = cross_val_score(svc_clf, X_train, y_train, cv=4)
```

5. As done in previous sections, view the average of the scores:

```
svc_scores.mean()

0.94795321637426899
```

6. Perform the same with support vector regression by importing SVR from `sklearn.svm`, the same module that contains SVC:

```
from sklearn.svm import SVR
```

7. Then write the necessary syntax to fit the model. It is almost identical to the syntax for SVC, just replacing some `c` keywords with `r`:

```
svr_clf = SVR(kernel = 'linear').fit(X_train, y_train)
```

Making a scorer

To make a scorer, you need:

- A scoring function that compares `y_test`, the ground truth, with `y_pred`, the predictions
- To determine whether a high score is good or bad

Before passing the SVR regressor to the cross-validation, make a scorer by supplying two elements:

8. In practice, begin by importing the `make_scorer` function:

```
from sklearn.metrics import make_scorer
```

9. Use this sample scoring function:

```
#Only works for this iris example with targets 0 and 1
def for_scorer(y_test, orig_y_pred):
    y_pred = np rint(orig_y_pred).astype(np.int)    #rounds
    prediction to the nearest integer
    return accuracy_score(y_test, y_pred)
```

The `np.rint` function rounds off the prediction to the nearest integer, hopefully one of the targets, 0 or 1. The `astype` method changes the type of the prediction to integer type, as the original target is in integer type and consistency is preferred with regard to types. After the rounding occurs, the scoring function uses the old `accuracy_score` function, which you are familiar with.

10. Now, determine whether a higher score is better. Higher accuracy is better, so for this situation, a higher score is better. In scikit code:

```
svr_to_class_scorer = make_scorer(for_scorer,
greater_is_better=True)
```

11. Finally, run the cross-validation with a new parameter, the scoring parameter:

```
svr_scores = cross_val_score(svr_clf, X_train, y_train, cv=4,
scoring = svr_to_class_scorer)
```

12. Find the mean:

```
svr_scores.mean()

0.94663742690058483
```

The accuracy scores are similar for the SVR regressor-based classifier and the traditional SVC classifier.

How it works...

You might ask, why did we take out class 2 out of the target set?

The reason is that, to use a regressor, our intent has to be to predict a real number. The categories had to have real number properties: that they are ordered (informally, if we have three ordered categories x , y , z and $x < y$ and $y < z$ then $x < z$). By eliminating the third category, the remaining flowers (Setosa and Versicolor) became ordered by a property we invented: Setosanness or Versicolorness.

The next time you encounter categories, you can consider whether they can be ordered. For example, if the dataset consists of shoe sizes, they can be ordered and a regressor can be applied, even though no one has a shoe size of 12.125.

There's more...

Linear versus nonlinear

Linear algorithms involve lines or hyperplanes. Hyperplanes are flat surfaces in any n -dimensional space. They tend to be easy to understand and explain, as they involve ratios (with an offset). Some functions that consistently and monotonically increase or decrease can be mapped to a linear function with a transformation. For example, exponential growth can be mapped to a line with the log transformation.

Nonlinear algorithms tend to be tougher to explain to colleagues and investors, yet ensembles of decision trees that are nonlinear tend to perform very well. KNN, which we examined earlier, is nonlinear. In some cases, functions not increasing or decreasing in a familiar manner are acceptable for the sake of accuracy.

Try a simple SVC with a polynomial kernel, as follows:

```
from sklearn.svm import SVC    #Usual import of SVC
svc_poly_clf = SVC(kernel = 'poly', degree= 3).fit(X_train, y_train)
#Polynomial Kernel of Degree 3
```

The polynomial kernel of degree 3 looks like a cubic curve in two dimensions. It leads to a slightly better fit, but note that it can be harder to explain to others than a linear kernel with consistent behavior throughout all of the Euclidean space:

```
svc_poly_scores = cross_val_score(svc_clf, X_train, y_train, cv=4)
svc_poly_scores.mean()
```

```
0.95906432748538006
```

Black box versus not

For the sake of efficiency, we did not examine the classification algorithms used very closely. When we compared SVC and logistic regression, we chose SVMs. At that point, both algorithms were black boxes, as we did not know any internal details. Once we decided to focus on SVMs, we could proceed to compute coefficients of the separating hyperplanes involved, optimize the hyperparameters of the SVM, use the SVM for big data, and do other processes. The SVMs have earned our time investment because of their superior performance.

Interpretability

Some machine learning algorithms are easier to understand than others. These are usually easier to explain to others as well. For example, linear regression is well known and easy to understand and explain to potential investors of your company. SVMs are more difficult to entirely understand.

My general advice: if SVMs are highly effective for a particular dataset, try to increase your personal interpretability of SVMs in the particular problem context. Also, consider merging algorithms somehow, using linear regression as an input to SVMs, for example. This way, you have the best of both worlds.

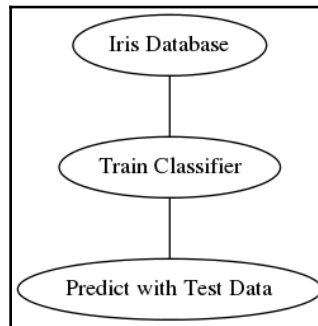


This is really context-specific, however. Linear SVMs are relatively simple to visualize and understand. Merging linear regression with SVM could complicate things. You can start by comparing them side by side.

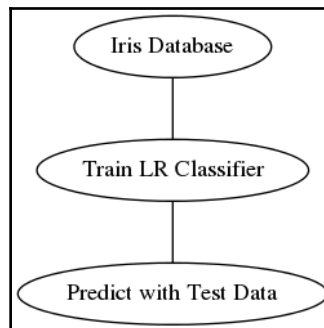
However, if you cannot understand every detail of the math and practice of SVMs, be kind to yourself, as machine learning is focused more on prediction performance rather than traditional statistics.

A pipeline

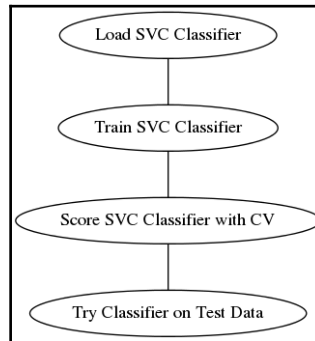
In programming, a pipeline is a set of procedures connected in series, one after the other, where the output of one process is the input to the next:



You can replace any procedure in the process with a different one, perhaps better in some way, without compromising the whole system. For the model in the middle step, you can use an SVC or logistic regression:



One can also keep track of the classifier itself and build a flow diagram from the classifier. Here is a pipeline keeping track of the SVC classifier:



In the upcoming chapters, we will see how scikit-learn uses the intuitive notion of a pipeline. So far, we have used a simple one: train, predict, test.

2

Pre-Model Workflow and Pre-Processing

In this chapter we will see the following recipes:

- Creating sample data for toy analysis
- Scaling data to the standard normal distribution
- Creating binary features through thresholding
- Working with categorical variables
- Imputing missing values through various strategies
- A linear model in the presence of outliers
- Putting it all together with pipelines
- Using Gaussian processes for regression
- Using SGD for regression

Introduction

What is data, and what are we doing with it?

A simple answer is that we attempt to place our data as points on paper, graph them, think, and look for simple explanations that approximate the data well. The simple geometric line of $F=ma$ (force being proportional to acceleration) explained a lot of noisy data for hundreds of years. I tend to think of data science as data compression at times.

Sometimes, when a machine is given only win-lose outcomes (of winning games of checkers, for example) and trained, I think of artificial intelligence. It is never taught explicit directions on how to play to win in such a case.

This chapter deals with the pre-processing of data in scikit-learn. Some questions you can ask about your dataset are as follows:

- Are there missing values in your dataset?
- Are there outliers (points far away from the others) in your set?
- What are the variables in the data like? Are they continuous quantities or categories?
- What do the continuous variable distributions look like? Can any of the variables in your dataset be described by normal distributions (bell-shaped curves)?
- Can any continuous variables be turned into categorical variables for simplicity? (This tends to be true if the distribution takes on very few particular values and not a continuous-like range of values.)
- What are the units of the variables involved? Will you mix the variables somehow in the machine learning algorithm you chose to use?

These questions can have simple or complex answers. Thankfully, you ask them many times, even on the same dataset, and after these recipes you will have some practice at crafting answers to pre-processing machine learning questions.

Additionally, we will see pipelines: a great organizational tool to make sure we perform the same operations on both the training and testing sets without errors and with relatively little work. We will also see regression examples: **stochastic gradient descent (SGD)** and Gaussian processes.

Creating sample data for toy analysis

If possible, use some of your own data for this book, but in the event you cannot, we'll learn how we can use scikit-learn to create toy data. scikit-learn's pseudo, theoretically constructed data is very interesting in its own right.

Getting ready

Very similar to getting built-in datasets, fetching new datasets, and creating sample datasets, the functions that are used follow the naming convention `make_*`. Just to be clear, this data is purely artificial:

```
from sklearn import datasets
datasets.make_*?

datasets.make_biclusters
```

```
datasets.make_blobs
datasets.make_checkerboard
datasets.make_circles
datasets.make_classification
...
```

To save typing, import the `datasets` module as `d`, and `numpy` as `np`:

```
import sklearn.datasets as d
import numpy as np
```

How to do it...

This section will walk you through the creation of several datasets. In addition to the sample datasets, these will be used throughout the book to create data with the necessary characteristics for the algorithms on display.

Creating a regression dataset

1. First, the stalwart—regression:

```
reg_data = d.make_regression()
```

By default, this will generate a tuple with a 100 × 100 matrix—100 samples by 100 features. However, by default, only 10 features are responsible for the target data generation. The second member of the tuple is the target variable. It is also possible to get more involved in generating data for regression.

2. For example, to generate a 1,000 × 10 matrix with five features responsible for the target creation, an underlying bias factor of 1.0, and 2 targets, the following command will be run:

```
complex_reg_data = d.make_regression(1000, 10, 5, 2, 1.0)
complex_reg_data[0].shape

(1000L, 10L)
```

Creating an unbalanced classification dataset

Classification datasets are also very simple to create. It's simple to create a base classification set, but the basic case is rarely experienced in practice—most users don't convert, most transactions aren't fraudulent, and so on.

3. Therefore, it's useful to explore classification on unbalanced datasets:

```
classification_set = d.make_classification(weights=[0.1])
np.bincount(classification_set[1])

array([10, 90], dtype=int64)
```

Creating a dataset for clustering

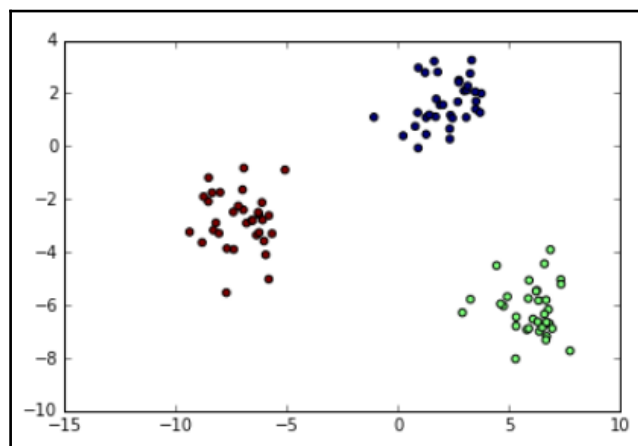
Clusters will also be covered. There are actually several functions to create datasets that can be modeled by different cluster algorithms.

4. For example, blobs are very easy to create and can be modeled by k-means:

```
blobs_data, blobs_target = d.make_blobs()
```

5. This will look like the following:

```
import matplotlib.pyplot as plt
%matplotlib inline
#Within an Ipython notebook
plt.scatter(blobs_data[:,0],blobs_data[:,1],c = blobs_target)
```



How it works...

Let's walk you through how scikit-learn produces the regression dataset by taking a look at the source code (with some modifications for clarity). Any undefined variables are assumed to have the default value of `make_regression`.

It's actually surprisingly simple to follow. First, a random array is generated with the size specified when the function is called:

```
x = np.random.randn(n_samples, n_features)
```

Given the basic dataset, the target dataset is then generated:

```
ground_truth = np.zeros((n_samples, n_target))
ground_truth[:n_informative, :] = 100*np.random.rand(n_informative,
n_targets)
```

The dot product of `x` and `ground_truth` are taken to get the final target values. Bias, if any, is added at this time:

```
y = np.dot(X, ground_truth) + bias
```

The dot product is simply a matrix multiplication. So, our final dataset will have `n_samples`, which is the number of rows from the dataset, and `n_target`, which is the number of target variables.

Due to NumPy's broadcasting, `bias` can be a scalar value, and this value will be added to every sample. Finally, it's a simple matter of adding any noise and shuffling the dataset. Voila, we have a dataset that's perfect for testing regression.

Scaling data to the standard normal distribution

A pre-processing step that is recommended is to scale columns to the standard normal. The standard normal is probably the most important distribution in statistics. If you've ever been introduced to statistics, you must have almost certainly seen z-scores. In truth, that's all this recipe is about—transforming our features from their endowed distribution into z-scores.

Getting ready

The act of scaling data is extremely useful. There are a lot of machine learning algorithms, which perform differently (and incorrectly) in the event the features exist at different scales. For example, SVMs perform poorly if the data isn't scaled because they use a distance function in their optimization, which is biased if one feature varies from 0 to 10,000 and the other varies from 0 to 1.

The preprocessing module contains several useful functions for scaling features:

```
from sklearn import preprocessing
import numpy as np # we'll need it later
```

Load the Boston dataset:

```
from sklearn.datasets import load_boston

boston = load_boston()
X,y = boston.data, boston.target
```

How to do it...

1. Continuing with the Boston dataset, run the following commands:

```
X[:, :3].mean(axis=0) #mean of the first 3 features

array([ 3.59376071, 11.36363636, 11.13677866])

X[:, :3].std(axis=0)

array([ 8.58828355, 23.29939569,  6.85357058])
```

2. There's actually a lot to learn from this initially. Firstly, the first feature has the smallest mean but varies even more than the third feature. The second feature has the largest mean and standard deviation—it takes the widest spread of values:

```
X_2 = preprocessing.scale(X[:, :3])
X_2.mean(axis=0)

array([ 6.34099712e-17, -6.34319123e-16, -2.68291099e-15])

X_2.std(axis=0)

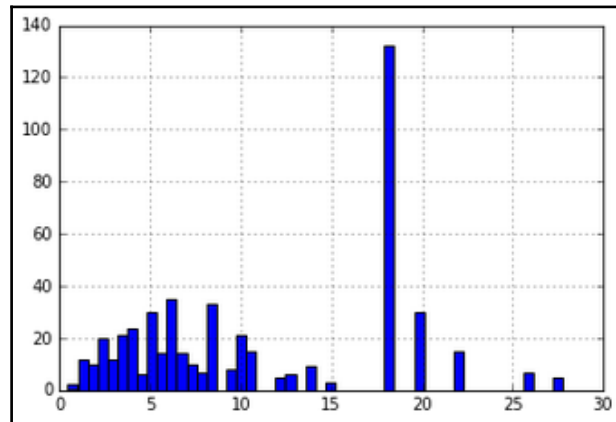
array([ 1., 1., 1.] )
```

How it works...

The centering and scaling function is extremely simple. It merely subtracts the mean and divides by the standard deviation.

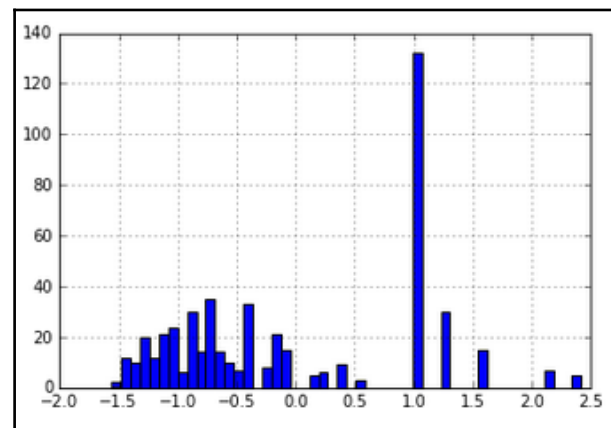
Pictorially and with pandas, the third feature looks as follows before the transformation:

```
pd.Series(X[:, 2]).hist(bins=50)
```



This is what it looks like afterward:

```
pd.Series(preprocessing.scale(X[:, 2])).hist(bins=50)
```



The x axis label has changed.

In addition to a function, there is also a centering and scaling class that is easy to invoke, and this is particularly useful when used in conjunction with pipelines, which are mentioned later. It's also useful for the centering and scaling class to persist across individual scaling:

```
my_scaler = preprocessing.StandardScaler()
my_scaler.fit(X[:, :3])
my_scaler.transform(X[:, :3]).mean(axis=0)

array([ 6.34099712e-17, -6.34319123e-16, -2.68291099e-15])
```

Scaling features to a mean of zero and a standard deviation of one isn't the only useful type of scaling.

Pre-processing also contains a `MinMaxScaler` class, which will scale the data within a certain range:

```
my_minmax_scaler = preprocessing.MinMaxScaler()
my_minmax_scaler.fit(X[:, :3])
my_minmax_scaler.transform(X[:, :3]).max(axis=0)

array([ 1.,  1.,  1.])

my_minmax_scaler.transform(X[:, :3]).min(axis=0)

array([ 0.,  0.,  0.])
```

It's very simple to change the minimum and maximum values of the `MinMaxScaler` class from its defaults of 0 and 1, respectively:

```
my_odd_scaler = preprocessing.MinMaxScaler(feature_range=(-3.14, 3.14))
```

Furthermore, another option is normalization. This will scale each sample to have a length of one. This is different from the other types of scaling done previously, where the features were scaled. Normalization is illustrated in the following command:

```
normalized_X = preprocessing.normalize(X[:, :3])
```

If it's not apparent why this is useful, consider the Euclidean distance (a measure of similarity) between three of the samples, where one sample has the values $(1, 1, 0)$, another has $(3, 3, 0)$, and the final has $(1, -1, 0)$.

The distance between the first and third vector is less than the distance between the first and second although the first and third are orthogonal, whereas the first and second only differ by a scalar factor of three. Since distances are often used as measures of similarity, not normalizing the data first can be misleading.

From an alternative perspective, try the following syntax:

```
(normalized_X * normalized_X).sum(axis = 1)

array([ 1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,  1.,
        1.,  1.
        ...])
```

All the rows are normalized and consist of vectors of length one. In three dimensions, all normalized vectors lie on the surface of a sphere centered at the origin. The information left is the direction of the vectors because, by definition, by normalizing you are dividing the vector by its length. Do always remember, though, that when performing this operation you have set an origin at $(0, 0, 0)$ and you have turned any row of data in the array into a vector relative to this origin.

Creating binary features through thresholding

In the last recipe, we looked at transforming our data into the standard normal distribution. Now, we'll talk about another transformation, one that is quite different. Instead of working with the distribution to standardize it, we'll purposely throw away data; if we have good reason, this can be a very smart move. Often, in what is ostensibly continuous data, there are discontinuities that can be determined via binary features.

Additionally, note that in the previous chapter, we turned a classification problem into a regression problem. With thresholding, we can turn a regression problem into a classification problem. This happens in some data science contexts.

Getting ready

Creating binary features and outcomes is a very useful method, but it should be used with caution. Let's use the Boston dataset to learn how to turn values into binary outcomes. First, load the Boston dataset:

```
import numpy as np
from sklearn.datasets import load_boston

boston = load_boston()
X, y = boston.data, boston.target.reshape(-1, 1)
```


How to do it...

Similar to scaling, there are two ways to binarize features in scikit-learn:

- `preprocessing.binarize`
- `preprocessing.Binarizer`

The Boston dataset's `target` variable is the median value of houses in thousands. This dataset is good for testing regression and other continuous predictors, but consider a situation where we want to simply predict whether a house's value is more than the overall mean.

1. To do this, we will want to create a threshold value of the mean. If the value is greater than the mean, produce a 1; if it is less, produce a 0:

```
from sklearn import preprocessing
new_target =
preprocessing.binarize(y, threshold=boston.target.mean())
new_target[:5]

array([[ 1.],
       [ 0.],
       [ 1.],
       [ 1.],
       [ 1.]])
```

2. This was easy, but let's check to make sure it worked correctly:

```
(y[:5] > y.mean()).astype(int)

array([[1],
       [0],
       [1],
       [1],
       [1]])
```

3. Given the simplicity of the operation in NumPy, it's a fair question to ask why you would want to use the built-in functionality of scikit-learn. Pipelines, covered in the *Putting it all together with pipelines* recipe, will help to explain this; in anticipation of this, let's use the `Binarizer` class:

```
binar = preprocessing.Binarizer(y.mean())
new_target = binar.fit_transform(y)
new_target[:5]
```

```
array([[ 1.],
       [ 0.],
       [ 1.],
       [ 1.],
       [ 1.]])
```

There's more...

Let's also learn about sparse matrices and the `fit` method.

Sparse matrices

Sparse matrices are special in that zeros aren't stored; this is done in an effort to save space in memory. This creates an issue for the binarizer, so to combat it, a special condition for the binarizer for sparse matrices is that the threshold cannot be less than zero:

```
from scipy.sparse import coo
spar = coo.coo_matrix(np.random.binomial(1, .25, 100))
preprocessing.binarize(spar, threshold=-1)
```

```
ValueError: Cannot binarize a sparse matrix with threshold < 0
```

The fit method

The `fit` method exists for the binarizer transformation, but it will not fit anything; it will simply return the object. The object, however, will store the threshold and be ready for the `transform` method.

Working with categorical variables

Categorical variables are a problem. On one hand they provide valuable information; on the other hand, it's probably text—either the actual text or integers corresponding to the text—such as an index in a lookup table.

So, we clearly need to represent our text as integers for the model's sake, but we can't just use the `id` field or naively represent them. This is because we need to avoid a similar problem to the *Creating binary features through thresholding* recipe. If we treat data that is continuous, it must be interpreted as continuous.

Getting ready

The Boston dataset won't be useful for this section. While it's useful for feature binarization, it won't suffice for creating features from categorical variables. For this, the iris dataset will suffice.

For this to work, the problem needs to be turned on its head. Imagine a problem where the goal is to predict the sepal width; in this case, the species of the flower will probably be useful as a feature.

How to do it...

1. Let's get the data sorted first:

```
from sklearn import datasets
import numpy as np
iris = datasets.load_iris()

X = iris.data
y = iris.target
```

2. Place `x` and `y`, all of the numerical data, side-by-side. Create an encoder with scikit-learn to handle the category of the `y` column:

```
from sklearn import preprocessing
cat_encoder = preprocessing.OneHotEncoder()
cat_encoder.fit_transform(y.reshape(-1,1)).toarray()[ :5]

array([[ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  0.,  0.]])
```

How it works...

The encoder creates additional features for each categorical variable, and the value returned is a sparse matrix. The result is a sparse matrix by definition; each row of the new features has 0 everywhere, except for the column whose value is associated with the feature's category. Therefore, it makes sense to store this data in a sparse matrix. The `cat_encoder` is now a standard scikit-learn model, which means that it can be used again:

```
cat_encoder.transform(np.ones((3, 1)).toarray())  
  
array([[ 0.,  1.,  0.],  
       [ 0.,  1.,  0.],  
       [ 0.,  1.,  0.]])
```

In the previous chapter, we turned a classification problem into a regression problem. Here, there are three columns:

- The first column is 1 if the flower is a Setosa and 0 otherwise
- The second column is 1 if the flower is a Versicolor and 0 otherwise
- The third column is 1 if the flower is a Virginica and 0 otherwise

Thus, we could use any of these three columns to create a regression similar to the one in the previous chapter; we will perform a regression to determine the degree of setoseness of a flower as a real number. The matching statement in classification is whether a flower is a Setosa one or not. This is the problem statement if we perform binary classification of the first column.

scikit-learn has the capacity for this type of multi-output regression. Compare it with multiclass classification. Let's try a simple one.

Import the ridge regression regularized linear model. It tends to be very well behaved because it is regularized. Instantiate a ridge regressor class:

```
from sklearn.linear_model import Ridge  
ridge_inst = Ridge()
```

Now import a multi-output regressor that takes the ridge regressor instance as an argument:

```
from sklearn.multioutput import MultiOutputRegressor  
multi_ridge = MultiOutputRegressor(ridge_inst, n_jobs=-1)
```

From earlier in this recipe, transform the target variable y to a three-part target variable, y_multi , with `OneHotEncoder()`. If X and y were part of a pipeline, the pipeline would transform the training and testing sets separately, and this is preferable:

```
from sklearn import preprocessing  
cat_encoder = preprocessing.OneHotEncoder()  
y_multi = cat_encoder.fit_transform(y.reshape(-1,1)).toarray()
```

Create training and testing sets:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y_multi, stratify=y,
random_state= 7)
```

Fit the multi-output estimator:

```
multi_ridge.fit(X_train, y_train)

MultiOutputRegressor(estimator=Ridge(alpha=1.0, copy_X=True,
fit_intercept=True, max_iter=None,
    normalize=False, random_state=None, solver='auto', tol=0.001),
    n_jobs=-1)
```

Predict the multi-output target on the testing set:

```
y_multi_pre = multi_ridge.predict(X_test)
y_multi_pre[:5]

array([[ 0.81689644,  0.36563058, -0.18252702],
       [ 0.95554968,  0.17211249, -0.12766217],
       [-0.01674023,  0.36661987,  0.65012036],
       [ 0.17872673,  0.474319  ,  0.34695427],
       [ 0.8792691  ,  0.14446485, -0.02373395]])
```

Use the `binarize` function from the previous recipe to turn each real number into the integers 0 or 1:

```
from sklearn import preprocessing
y_multi_pred = preprocessing.binarize(y_multi_pre, threshold=0.5)
y_multi_pred[:5]

array([[ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 0.,  0.,  1.],
       [ 0.,  0.,  0.],
       [ 1.,  0.,  0.]])
```

We can measure the overall multi-output performance with the `roc_auc_score`:

```
from sklearn.metrics import roc_auc_score

roc_auc_score(y_test, y_multi_pre)
```

```
0.91987179487179482
```

Or, we can do it flower type by flower type, column by column:

```
from sklearn.metrics import accuracy_score

print ("Multi-Output Scores for the Iris Flowers: ")
for column_number in range(0,3):
    print ("Accuracy score of flower " +
str(column_number), accuracy_score(y_test[:,column_number],
y_multi_pred[:,column_number]))
    print ("AUC score of flower " +
str(column_number), roc_auc_score(y_test[:,column_number],
y_multi_pre[:,column_number]))
    print ("")

Multi-Output Scores for the Iris Flowers:
('Accuracy score of flower 0', 1.0)
('AUC score of flower 0', 1.0)

('Accuracy score of flower 1', 0.73684210526315785)
('AUC score of flower 1', 0.76923076923076927)

('Accuracy score of flower 2', 0.97368421052631582)
('AUC score of flower 2', 0.99038461538461542)
```

There's more...

In the preceding multi-output regression, you could be concerned with the dummy variable trap: the collinearity of the outputs. Without dropping any output columns, you assume that there is a fourth option: that a flower can be of none of the three types. To prevent the trap, drop the last column and assume that the flower has to be of one of the three types as we do not have any training examples where it is not one of the three flower types.

There are other ways to create categorical variables in scikit-learn and Python. The `DictVectorizer` class is a good option if you like to limit the dependencies of your projects to only scikit-learn and you have a fairly simple encoding scheme. However, if you require more sophisticated categorical encoding, `patsy` is a very good option.

DictVectorizer class

Another option is to use `DictVectorizer` class. This can be used to directly convert strings to features:

```
from sklearn.feature_extraction import DictVectorizer
dv = DictVectorizer()
my_dict = [{'species': iris.target_names[i]} for i in y]
dv.fit_transform(my_dict).toarray()[ :5]

array([[ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  0.,  0.],
       [ 1.,  0.,  0.]])
```

Imputing missing values through various strategies

Data imputation is critical in practice, and thankfully there are many ways to deal with it. In this recipe, we'll look at a few of the strategies. However, be aware that there might be other approaches that fit your situation better.

This means scikit-learn comes with the ability to perform fairly common imputations; it will simply apply some transformations to the existing data and fill the NAs. However, if the dataset is missing data, and there's a known reason for this missing data—for example, response times for a server that times out after 100 ms—it might be better to take a statistical approach through other packages, such as the Bayesian treatment via PyMC, hazards models via Lifelines, or something home-grown.

Getting ready

The first thing to do when learning how to input missing values is to create missing values. NumPy's masking will make this extremely simple:

```
from sklearn import datasets
import numpy as np

iris = datasets.load_iris()
iris_X = iris.data
masking_array = np.random.binomial(1, .25, iris_X.shape).astype(bool)
```

```
iris_X[masking_array] = np.nan
```

To unravel this a bit, in case NumPy isn't too familiar, it's possible to index arrays with other arrays in NumPy. So, to create the random missing data, a random Boolean array is created, which is of the same shape as the iris dataset. Then, it's possible to make an assignment via the masked array. It's important to note that because a random array is used, it is likely that your `masking_array` will be different from what's used here.

To make sure this works, use the following command (since we're using a random mask, it might not match directly):

```
masking_array[:5]

array([[ True, False, False,  True],
       [False, False, False, False],
       [False, False, False, False],
       [ True, False, False, False],
       [False, False, False,  True]], dtype=bool)

iris_X [:5]

array([[ nan,  3.5,  1.4,  nan],
       [ 4.9,  3. ,  1.4,  0.2],
       [ 4.7,  3.2,  1.3,  0.2],
       [ nan,  3.1,  1.5,  0.2],
       [ 5. ,  3.6,  1.4,  nan]])
```

How to do it...

1. A theme prevalent throughout this book (due to the theme throughout scikit-learn) is reusable classes that fit and transform datasets that can subsequently be used to transform unseen datasets. This is illustrated as follows:

```
from sklearn import preprocessing
impute = preprocessing.Imputer()
iris_X_prime = impute.fit_transform(iris_X)
iris_X_prime[:5]

array([[ 5.82616822,  3.5      ,  1.4      ,  1.22589286],
       [ 4.9      ,  3.      ,  1.4      ,  0.2      ],
       [ 4.7      ,  3.2     ,  1.3      ,  0.2      ],
       [ 5.82616822,  3.1      ,  1.5      ,  0.2      ],
       [ 5.      ,  3.6      ,  1.4      ,  1.22589286]])
```


2. Notice the difference in the position [0, 0]:

```
iris_X_prime[0, 0]

5.8261682242990664

iris_X[0, 0]

nan
```

How it works...

The imputation works by employing different strategies. The default is mean, but in total there are the following:

- mean (default)
- median
- most_frequent (mode)

scikit-learn will use the selected strategy to calculate the value for each non-missing value in the dataset. It will then simply fill the missing values. For example, to redo the iris example with the median strategy, simply reinitialize impute with the new strategy:

```
impute = preprocessing.Imputer(strategy='median')
iris_X_prime = impute.fit_transform(iris_X)
iris_X_prime[:5]

array([[ 5.8,  3.5,  1.4,  1.3],
       [ 4.9,  3. ,  1.4,  0.2],
       [ 4.7,  3.2,  1.3,  0.2],
       [ 5.8,  3.1,  1.5,  0.2],
       [ 5. ,  3.6,  1.4,  1.3]])
```

If the data is missing values, it might be inherently dirty in other places. For instance, in the example in the preceding, *How to do it...* section, `np.nan` (the default missing value) was used as the missing value, but missing values can be represented in many ways. Consider a situation where missing values are `-1`. In addition to the strategy to compute the missing value, it's also possible to specify the missing value for the imputer. The default is `nan`, which will handle `np.nan` values.

To see an example of this, modify `iris_X` to have `-1` as the missing value. It sounds crazy, but since the iris dataset contains measurements that are always possible, many people will fill the missing values with `-1` to signify they're not there:

```
iris_X[np.isnan(iris_X)] = -1
iris_X[:5]
```

Filling these in is as simple as the following:

```
impute = preprocessing.Imputer(missing_values=-1)
iris_X_prime = impute.fit_transform(iris_X)
iris_X_prime[:5]

array([[ 5.1 ,  3.5 ,  1.4 ,  0.2 ],
       [ 4.9 ,  3. ,  1.4 ,  0.2 ],
       [ 4.7 ,  3.2 ,  1.3 ,  0.2 ],
       [ 5.87923077,  3.1 ,  1.5 ,  0.2 ],
       [ 5. ,  3.6 ,  1.4 ,  0.2 ]])
```

There's more...

Pandas also provides a functionality to fill in missing data. It actually might be a bit more flexible, but it is less reusable:

```
import pandas as pd
iris_X_prime = np.where(pd.DataFrame(iris_X).isnull(), -1, iris_X)
iris_X_prime[:5]

array([[ -1. ,  3.5,  1.4, -1. ],
       [ 4.9,  3. ,  1.4,  0.2],
       [ 4.7,  3.2,  1.3,  0.2],
       [ -1. ,  3.1,  1.5,  0.2],
       [ 5. ,  3.6,  1.4, -1. ]])
```

To mention its flexibility, `fillna` can be passed any sort of statistic, that is, the strategy is more arbitrarily defined:

```
pd.DataFrame(iris_X).fillna(-1)[:5].values

array([[ -1. ,  3.5,  1.4, -1. ],
       [ 4.9,  3. ,  1.4,  0.2],
       [ 4.7,  3.2,  1.3,  0.2],
       [ -1. ,  3.1,  1.5,  0.2],
       [ 5. ,  3.6,  1.4, -1. ]])
```

A linear model in the presence of outliers

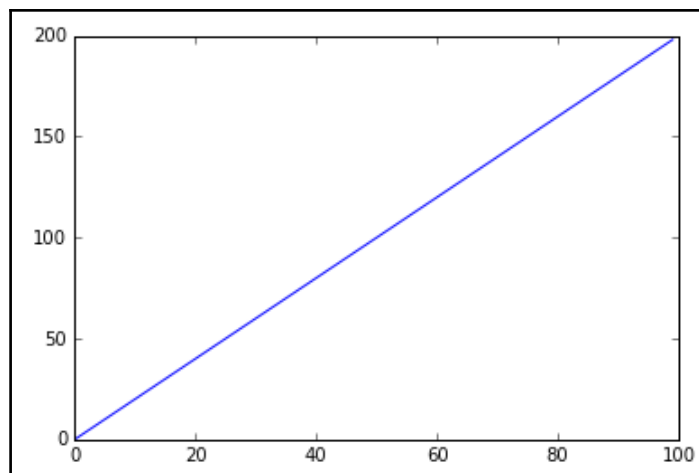
In this recipe, instead of traditional linear regression we will try using the Theil-Sen estimator to deal with some outliers.

Getting ready

First, create the data corresponding to a line with a slope of 2:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

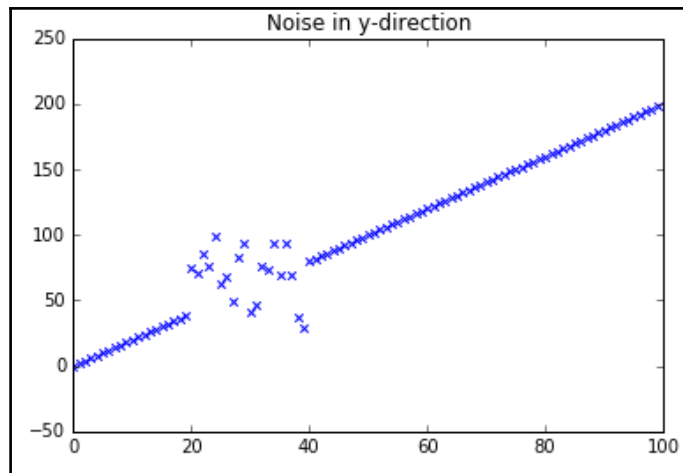
num_points = 100
x_vals = np.arange(num_points)
y_truth = 2 * x_vals
plt.plot(x_vals, y_truth)
```



Add noise to that data and label it as `y_noisy`:

```
y_noisy = y_truth.copy()
#Change y-values of some points in the line
y_noisy[20:40] = y_noisy[20:40] * (-4 * x_vals[20:40]) - 100

plt.title("Noise in y-direction")
plt.xlim([0,100])
plt.scatter(x_vals, y_noisy, marker='x')
```



How to do it...

1. Import both `LinearRegression` and `TheilSenRegressor`. Score the estimators using the original line as the testing set, `y_truth`:

```
from sklearn.linear_model import LinearRegression,
TheilSenRegressor
from sklearn.metrics import r2_score, mean_absolute_error

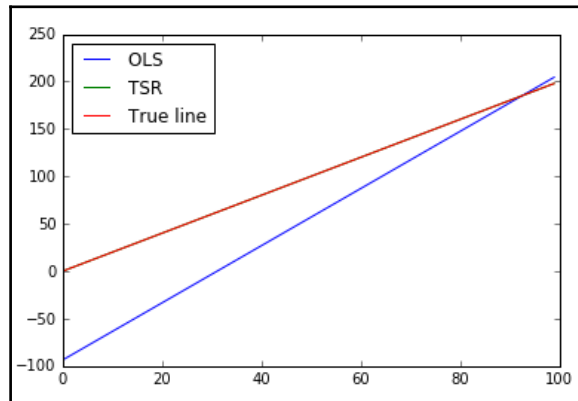
named_estimators = [('OLS ', LinearRegression()), ('TSR ',
TheilSenRegressor())]

for num_index, est in enumerate(named_estimators):
    y_pred = est[1].fit(x_vals.reshape(-1,
1), y_noisy).predict(x_vals.reshape(-1, 1))
    print (est[0], "R-squared: ", r2_score(y_truth, y_pred), "Mean
Absolute Error", mean_absolute_error(y_truth, y_pred))
    plt.plot(x_vals, y_pred, label=est[0])

('OLS ', 'R-squared: ', 0.17285546630270587, 'Mean Absolute
Error', 44.099173357335729)
('TSR ', 'R-squared: ', 0.99999999928066519, 'Mean Absolute
Error', 0.0013976236426276058)
```

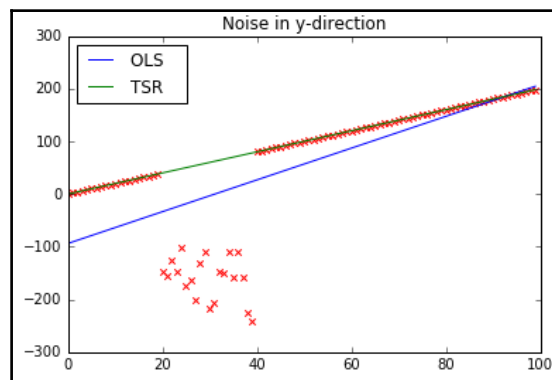
2. Plot the lines. Note that **ordinary least squares (OLS)** is way off the true line, `y_truth`. Theil-Sen overlaps the real line:

```
plt.plot(x_vals, y_truth, label='True line')
plt.legend(loc='upper left')
```



3. Plot the dataset and the estimated lines:

```
for num_index, est in enumerate(named_estimators):
    y_pred = est[1].fit(x_vals.reshape(-1,
1), y_noisy).predict(x_vals.reshape(-1, 1))
    plt.plot(x_vals, y_pred, label=est[0])
plt.legend(loc='upper left')
plt.title("Noise in y-direction")
plt.xlim([0,100])
plt.scatter(x_vals, y_noisy, marker='x', color='red')
```



How it works...

The `TheilSenRegressor` is a robust estimator that performs well in the presence of outliers. It uses the measurement of medians, which is more robust to outliers. In OLS regression, errors are squared, and thus a squared error can decrease good results.

You can try several robust estimators in scikit-learn Version 0.19.0:

```
from sklearn.linear_model import Ridge, LinearRegression,
TheilSenRegressor, RANSACRegressor, ElasticNet, HuberRegressor
from sklearn.metrics import r2_score, mean_absolute_error
named_estimators = [('OLS ', LinearRegression()),
('Ridge ', Ridge()), ('TSR ', TheilSenRegressor()), ('RANSAC',
RANSACRegressor()), ('ENet ', ElasticNet()), ('Huber ', HuberRegressor())]

for num_index, est in enumerate(named_estimators):
    y_pred = est[1].fit(x_vals.reshape(-1,
1), y_noisy).predict(x_vals.reshape(-1, 1))
    print (est[0], "R-squared: ", r2_score(y_truth, y_pred), "Mean Absolute
Error", mean_absolute_error(y_truth, y_pred))

('OLS ', 'R-squared: ', 0.17285546630270587, 'Mean Absolute Error',
44.099173357335729)
('Ridge ', 'R-squared: ', 0.17287378039132695, 'Mean Absolute Error',
44.098937961740631)
('TSR ', 'R-squared: ', 0.99999999928066519, 'Mean Absolute Error',
0.0013976236426276058)
('RANSAC', 'R-squared: ', 1.0, 'Mean Absolute Error',
1.0236256287043944e-14)
('ENet ', 'R-squared: ', 0.17407294649885618, 'Mean Absolute Error',
44.083506446776603)
('Huber ', 'R-squared: ', 0.9999999999404421, 'Mean Absolute Error',
0.00011755074198335526)
```

As you can see, the robust linear estimators Theil-Sen, **random sample consensus (RANSAC)**, and the Huber regressor out-perform the other linear regressors in the presence of outliers.

Putting it all together with pipelines

Now that we've used pipelines and data transformation techniques, we'll walk through a more complicated example that combines several of the previous recipes into a pipeline.

Getting ready

In this section, we'll show off some more of pipeline's power. When we used it earlier to impute missing values, it was only a quick taste; here, we'll chain together multiple pre-processing steps to show how pipelines can remove extra work.

Let's briefly load the iris dataset and seed it with some missing values:

```
from sklearn.datasets import load_iris
from sklearn.datasets import load_iris
import numpy as np
iris = load_iris()
iris_data = iris.data
mask = np.random.binomial(1, .25, iris_data.shape).astype(bool)
iris_data[mask] = np.nan
iris_data[:5]

array([[ nan,  3.5,  1.4,  0.2],
       [ 4.9,  3. ,  1.4,  nan],
       [ nan,  3.2,  nan,  nan],
       [ nan,  nan,  1.5,  0.2],
       [ nan,  3.6,  1.4,  0.2]])
```

How to do it...

The goal of this chapter is to first impute the missing values of `iris_data`, and then perform PCA on the corrected dataset. You can imagine (and we'll do it later) that this workflow might need to be split between a training dataset and a holdout set; pipelines will make this easier, but first we need to take a baby step.

1. Let's load the required libraries:

```
from sklearn import pipeline, preprocessing, decomposition
```

2. Next, create the `imputer` and `pca` classes:

```
pca = decomposition.PCA()
imputer = preprocessing.Imputer()
```

3. Now that we have the classes we need, we can load them into Pipeline:

```
pipe = pipeline.Pipeline([('imputer', imputer), ('pca', pca)])
iris_data_transformed = pipe.fit_transform(iris_data)
iris_data_transformed[:5]

array([[ -2.35980262,  0.6490648 ,  0.54014471,  0.00958185],
       [ -2.29755917, -0.00726168, -0.72879348, -0.16408532],
       [ -0.00991161,  0.03354407,  0.01597068,  0.12242202],
       [ -2.23626369,  0.50244737,  0.50725722, -0.38490096],
       [ -2.36752684,  0.67520604,  0.55259083,  0.1049866 ]])
```

This takes a lot more management if we use separate steps. Instead of each step requiring a fit transform, this step is performed only once, not to mention that we only have to keep track of one object!

How it works...

Hopefully it was obvious, but each step in a pipeline is passed to a pipeline object via a list of tuples, with the first element getting the name and the second getting the actual object. Under the hood, these steps are looped through when a method such as `fit_transform` is called on the pipeline object.

This said, there are quick and dirty ways to create a pipeline, much in the same way there was a quick way to perform scaling, though we can use `StandardScaler` if we want more power. The `pipeline` function will automatically create the names for the pipeline objects:

```
pipe2 = pipeline.make_pipeline(imputer, pca)
pipe2.steps

[('imputer',
  Imputer(axis=0, copy=True, missing_values='NaN', strategy='mean',
  verbose=0)),
 ('pca',
  PCA(copy=True, iterated_power='auto', n_components=None,
  random_state=None,
  svd_solver='auto', tol=0.0, whiten=False))]
```

This is the same object that was created in the more verbose method:

```
iris_data_transformed2 = pipe2.fit_transform(iris_data)
iris_data_transformed2[:5]

array([[ -2.35980262,  0.6490648 ,  0.54014471,  0.00958185],
       [ -2.29755917, -0.00726168, -0.72879348, -0.16408532],
```



```
[-0.00991161,  0.03354407,  0.01597068,  0.12242202],
[-2.23626369,  0.50244737,  0.50725722, -0.38490096],
[-2.36752684,  0.67520604,  0.55259083,  0.1049866  ]]
```

There's more...

We just walked through pipelines at a very high level, but it's unlikely that we will want to apply the base transformation. Therefore, the attributes of each object in a pipeline can be accessed using a `set_params` method, where the parameter follows the `<step_name>__<step_parameter>` convention. For example, let's change the `pca` object to use two components:

```
pipe2.set_params(pca__n_components=2)

Pipeline(steps=[('imputer', Imputer(axis=0, copy=True,
missing_values='NaN', strategy='mean', verbose=0)), ('pca', PCA(copy=True,
iterated_power='auto', n_components=2, random_state=None,
svd_solver='auto', tol=0.0, whiten=False))])
```

Notice, `n_components=2` in the preceding output. Just as a test, we can output the same transformation we have already done twice, and the output will be an $N \times 2$ matrix:

```
iris_data_transformed3 = pipe2.fit_transform(iris_data)
iris_data_transformed3[:5]

array([[-2.35980262,  0.6490648 ],
       [-2.29755917, -0.00726168],
       [-0.00991161,  0.03354407],
       [-2.23626369,  0.50244737],
       [-2.36752684,  0.67520604]])
```

Using Gaussian processes for regression

In this recipe, we'll use a Gaussian process for regression. In the linear models section, we will see how representing prior information on the coefficients was possible using Bayesian ridge regression.

With a Gaussian process, it's about the variance and not the mean. However, with a Gaussian process, we assume the mean is 0, so it's the covariance function we'll need to specify.

The basic setup is similar to how a prior can be put on the coefficients in a typical regression problem. With a Gaussian process, a prior can be put on the functional form of the data, and it's the covariance between the data points that is used to model the data, and therefore, must fit the data.

A big advantage of Gaussian processes is that they can predict probabilistically: you can obtain confidence bounds on your predictions. Additionally, the prediction can interpolate the observations for the available kernels: predictions from regression are smooth and thus a prediction between two points you know about is between those two points.

A disadvantage of Gaussian processes is lack of efficiency in high-dimensional spaces.

Getting ready

So, let's use some regression data and walk through how Gaussian processes work in scikit-learn:

```
from sklearn.datasets import load_boston
boston = load_boston()
boston_X = boston.data
boston_y = boston.target
train_set = np.random.choice([True, False], len(boston_y), p=[.75, .25])
```

How to do it...

1. We have the data, we'll create a scikit-learn `GaussianProcessRegressor` object. Let's look at the `gpr` object:

```
sklearn.gaussian_process import GaussianProcessRegressor
gpr = GaussianProcessRegressor()
gpr

GaussianProcessRegressor(alpha=1e-10, copy_X_train=True,
kernel=None,
n_restarts_optimizer=0, normalize_y=False,
optimizer='fmin_l_bfgs_b', random_state=None)
```

There are a few parameters that are important and must be set:

- `alpha`: This is a noise parameter. You can assign a noise value for all observations or assign `n` values in the form of a NumPy array where `n` is the length of the target observations in the training set you pass to `gpr` for training.
- `kernel`: This is a kernel that approximates a function. The default in a previous version of scikit-learn was **radial basis functions (RBF)**, and we will construct a flexible kernel from constant kernels and RBF kernels.
- `normalize_y`: You can set it to true if the mean of the target set is not zero. If you leave it set to false, it still works fairly well.
- `n_restarts_optimizer`: Set this to 10-20 for practical use. This is the number of iterations to optimize the kernel.

2. Import the required kernel functions and set a flexible kernel:

```
from sklearn.gaussian_process.kernels import RBF, ConstantKernel as CK

mixed_kernel = kernel = CK(1.0, (1e-4, 1e4)) * RBF(10, (1e-4, 1e4))
```

3. Finally, instantiate and fit the algorithm. Note that `alpha` is set to 5 for all values. I came up with that number as being around one-fourth of the target values:

```
gpr = GaussianProcessRegressor(alpha=5,
                               n_restarts_optimizer=20,
                               kernel = mixed_kernel)

gpr.fit(boston_X[train_set], boston_y[train_set])
```

4. Store the predictions on unseen data as `test_preds`:

```
test_preds = gpr.predict(boston_X[~train_set])
```

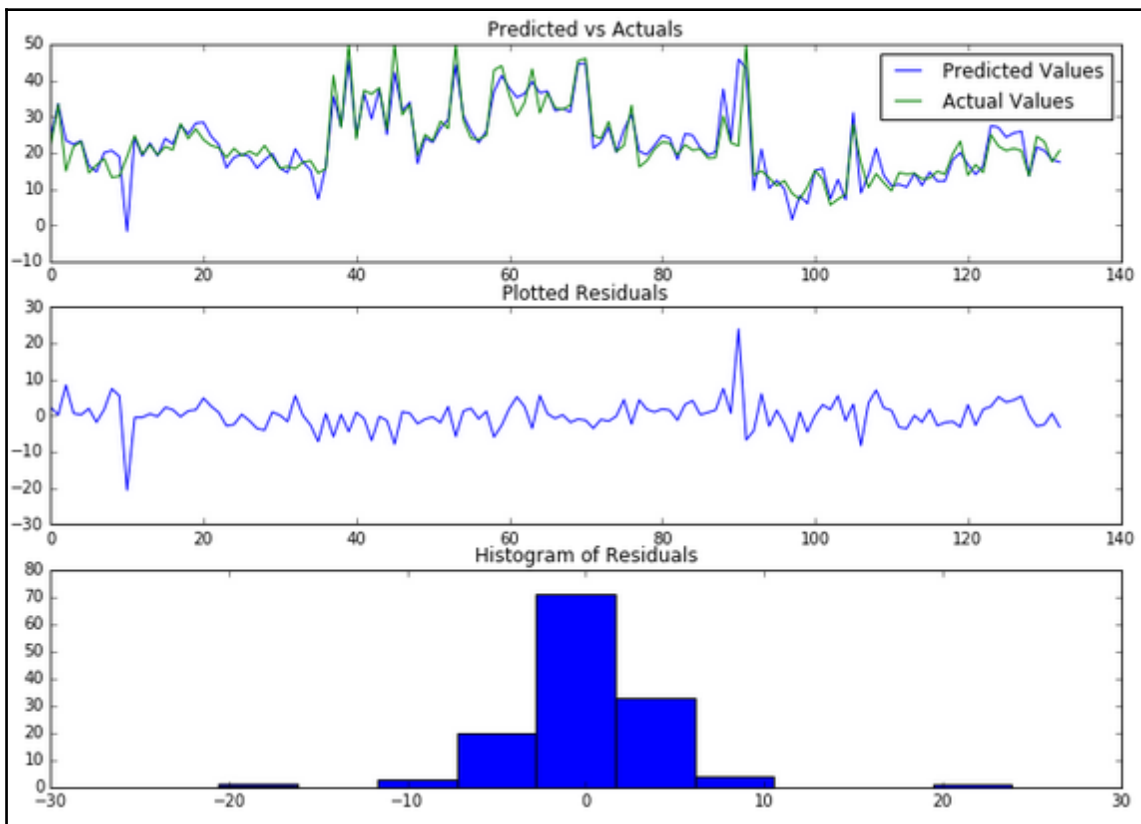
5. Plot the results:

```
>from sklearn.model_selection import cross_val_predict

from matplotlib import pyplot as plt
%matplotlib inline

f, ax = plt.subplots(figsize=(10, 7), nrows=3)
f.tight_layout()
```

```
ax[0].plot(range(len(test_preds)), test_preds, label='Predicted  
Values');  
ax[0].plot(range(len(test_preds)),  
boston_y[~train_set], label='Actual Values');  
ax[0].set_title("Predicted vs Actuals")  
ax[0].legend(loc='best')  
  
ax[1].plot(range(len(test_preds)), test_preds -  
boston_y[~train_set]);  
ax[1].set_title("Plotted Residuals")  
ax[2].hist(test_preds - boston_y[~train_set]);  
ax[2].set_title("Histogram of Residuals")
```



Cross-validation with the noise parameter

You might wonder if that is the best noise parameter, $\alpha=5$? To figure this out, try some cross-validation.

1. First, produce a cross-validation score with $\alpha=5$. Note the scorer within the `cross_val_score` object is `neg_mean_absolute_error`, as the default R-squared score is hard to read for this dataset:

```
from sklearn.model_selection import cross_val_score

gpr5 = GaussianProcessRegressor(alpha=5,
                                n_restarts_optimizer=20,
                                kernel = mixed_kernel)

scores_5 = (cross_val_score(gpr5,
                             boston_X[train_set],
                             boston_y[train_set],
                             cv = 4,
                             scoring = 'neg_mean_absolute_error'))
```

2. Look at the scores in `scores_5`:

```
def score_mini_report(scores_list):
    print "List of scores: ", scores_list
    print "Mean of scores: ", scores_list.mean()
    print "Std of scores: ", scores_list.std()
    score_mini_report(scores_5)

List of scores:  [ -4.10973995  -4.93446898  -3.78162
-13.94513686]
Mean of scores:  -6.69274144767
Std of scores:   4.20818506589
```

Observe that the scores in the last fold do not look the same as the other three.

3. Now produce a report with $\alpha=7$:

```
gpr7 = GaussianProcessRegressor(alpha=7,
                                n_restarts_optimizer=20,
                                kernel = mixed_kernel)

scores_7 = (cross_val_score(gpr7,
                             boston_X[train_set],
                             boston_y[train_set],
                             cv = 4,
                             scoring = 'neg_mean_absolute_error'))
```

```
score_mini_report(scores_7)
```

```
List of scores:  [-3.70606009 -4.92211642 -3.63887969
-14.20478333]
```

```
Mean of scores:  -6.61795988295
```

```
Std of scores:   4.40992783912
```

4. This score looks a little better. Now, try `alpha=7` and `normalize_y` set to `True`:

```
from sklearn.model_selection import cross_val_score
```

```
gpr7n = GaussianProcessRegressor(alpha=7,
                                n_restarts_optimizer=20,
                                kernel = mixed_kernel,
                                normalize_y=True)
```

```
scores_7n = (cross_val_score(gpr7n,
                              boston_X[train_set],
                              boston_y[train_set],
                              cv = 4,
                              scoring = 'neg_mean_absolute_error'))
```

```
score_mini_report(scores_7n)
```

```
List of scores:  [-4.0547601 -4.91077385 -3.65226736 -9.05596047]
```

```
Mean of scores:  -5.41844044809
```

```
Std of scores:   2.1487361839
```

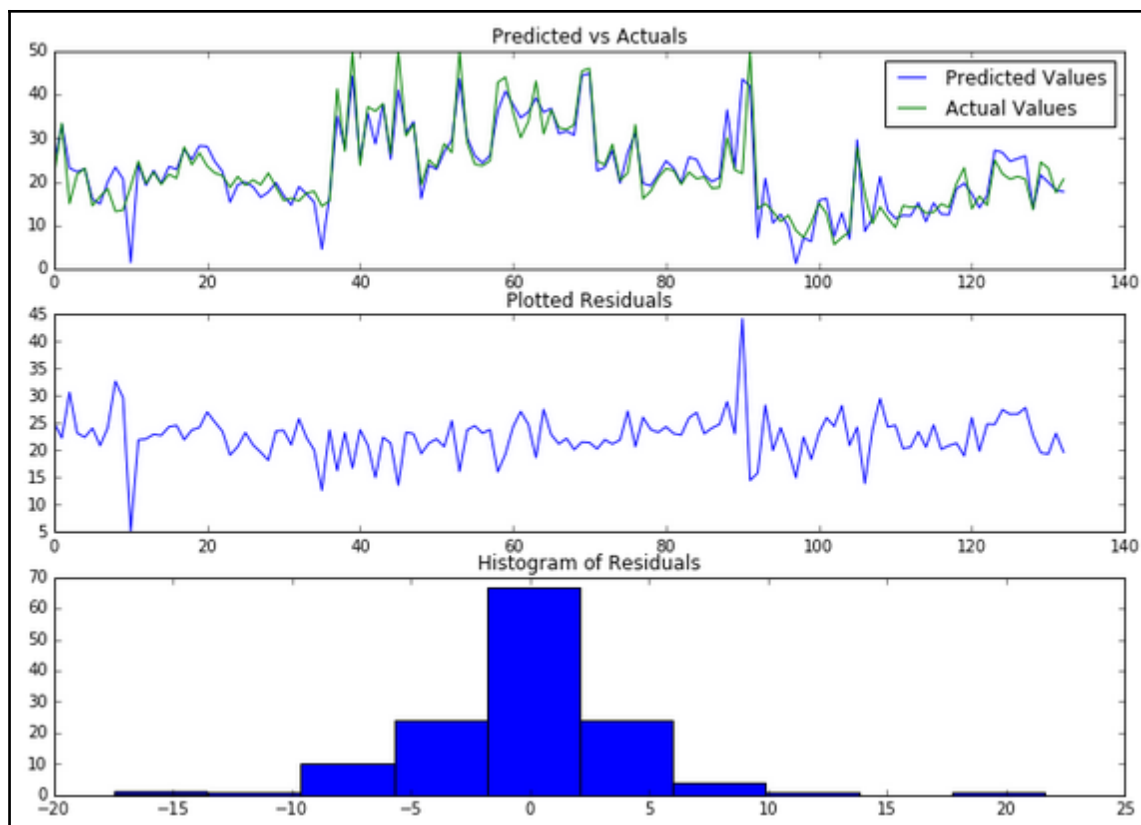
5. This looks even better, as the mean is higher and the standard deviation is lower. Let's select the last model for final training:

```
gpr7n.fit(boston_X[train_set], boston_y[train_set])
```

6. Predict it:

```
test_preds = gpr7n.predict(boston_X[~train_set])
```

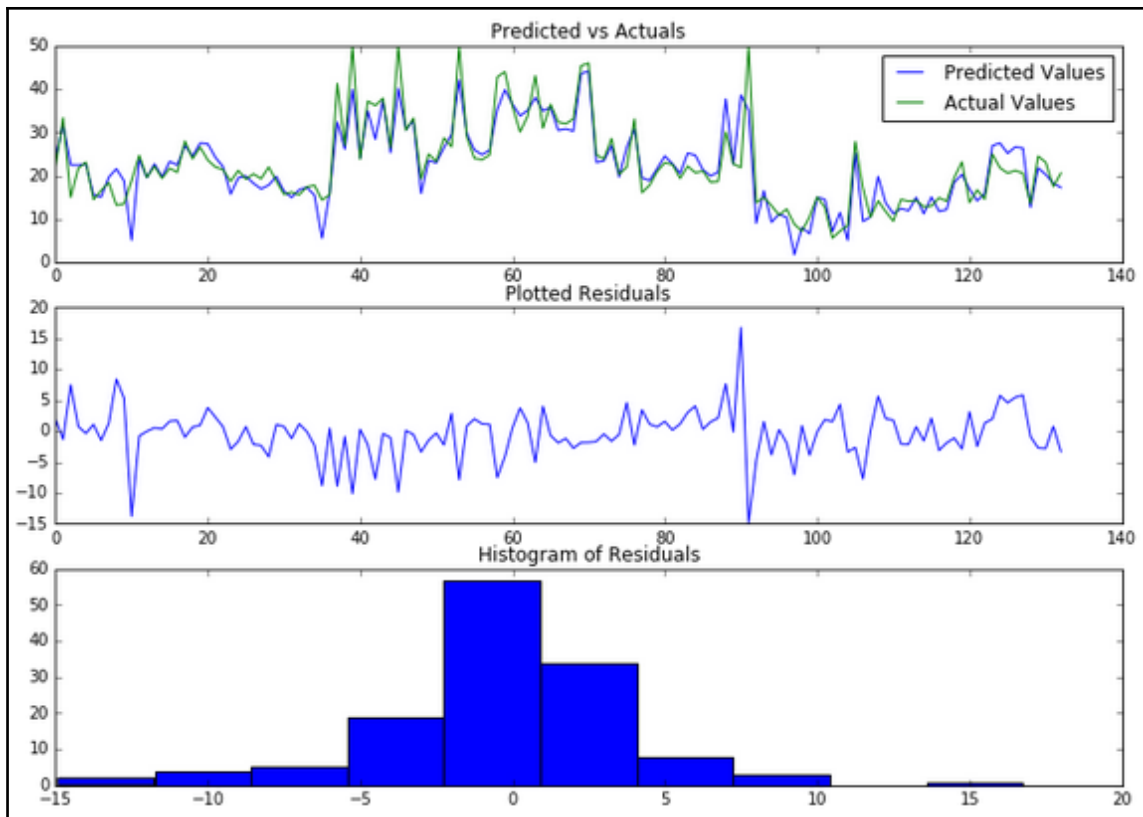
7. Visualize the results:



8. The residuals look a bit more centered. You can also pass a NumPy array for alpha:

```
gpr_new = GaussianProcessRegressor(alpha=boston_y[train_set]/4,  
                                   n_restarts_optimizer=20,  
                                   kernel = mixed_kernel)
```

9. This leads to the following graphs:



The array `alphas` are not compatible with `cross_val_score`, so I cannot select this model as the best model by looking at the final graphs and deciding which is the best. So, our final model selection is `gpr7n` with `alpha=7` and `normalize_y=True`.

There's more...

Underneath it all, the kernel computes covariances between points in x . It assumes that similar points in the inputs should lead to similar outputs. Gaussian processes are great for confidence predictions and smooth-like outputs. (Later, we will see random forests, that do not lead to smooth outputs even though they are very predictive.)

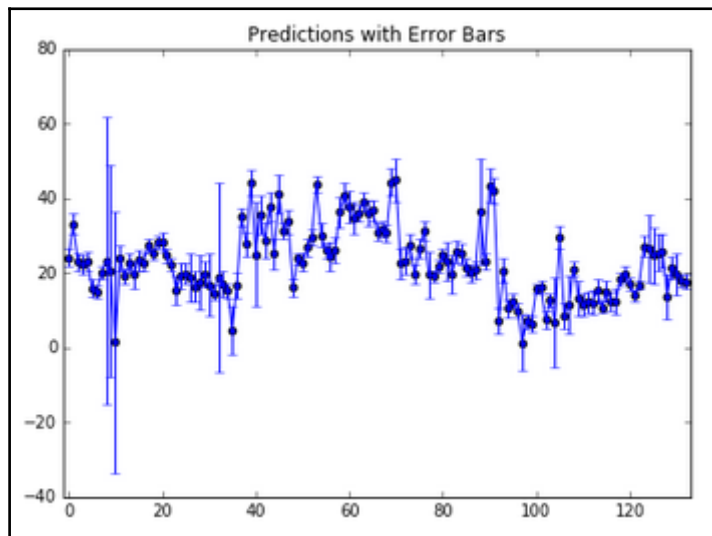
We may need to understand the uncertainty in our estimates. If we pass the `eval_MSE` argument as true, we'll get MSE and the predicted values, so we can make the predictions. A tuple of predictions and MSE is returned, from a mechanics standpoint:

```
test_preds, MSE = gpr7n.predict(boston_X[~train_set], return_std=True)
MSE[:5]

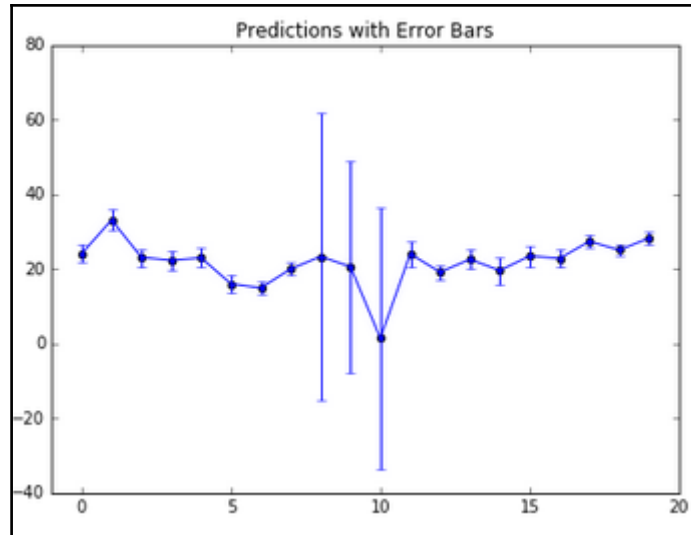
array([ 1.20337425,  1.43876578,  1.19910262,  1.35212445,  1.32769539])
```

Plot all of the predictions with error bars as follows:

```
f, ax = plt.subplots(figsize=(7, 5))
n = 133
rng = range(n)
ax.scatter(rng, test_preds[:n])
ax.errorbar(rng, test_preds[:n], yerr=1.96*MSE[:n])
ax.set_title("Predictions with Error Bars")
ax.set_xlim((-1, n));
```



Set $n=20$ in the preceding code to look at fewer points:



The uncertainty is very high for some points. As you can see, there is a lot of variance in the estimates for many of the given points. However, the overall error is not that bad.

Using SGD for regression

In this recipe, we'll get our first taste of stochastic gradient descent. We'll use it for regression here.

Getting ready

SGD is often an unsung hero in machine learning. Underneath many algorithms, there is SGD doing the work. It's popular due to its simplicity and speed—these are both very good things to have when dealing with a lot of data. The other nice thing about SGD is that while it's at the core of many machine learning algorithms computationally, it does so because it easily describes the process. At the end of the day, we apply some transformation on the data, and then we fit our data to the model with a loss function.

How to do it...

1. If SGD is good on large datasets, we should probably test it on a fairly large dataset:

```
from sklearn.datasets import make_regression
X, y = make_regression(int(1e6)) #1,000,000 rows
```

It's probably worth gaining some intuition about the composition and size of the object. Thankfully, we're dealing with NumPy arrays, so we can just access `nbytes`. The built-in Python way to access the object's size doesn't work for NumPy arrays.

2. This output can be system dependent, so you may not get the same results:

```
print "{:,}".format(X.nbytes)

800,000,000
```

3. To get some human perspective, we can convert `nbytes` to megabytes. There are roughly 1 million bytes in a megabyte:

```
X.nbytes / 1e6

800
```

4. So, the number of bytes per data point is as follows:

```
X.nbytes / (X.shape[0]*X.shape[1])

8
```

Well, isn't that tidy, and fairly tangential, for what we're trying to accomplish? However, it's worth knowing how to get the size of the objects you're dealing with.

5. So, now that we have the data, we can simply fit a `SGDRegressor`:

```
from sklearn.linear_model import SGDRegressor
sgd = SGDRegressor()
train = np.random.choice([True, False], size=len(y), p=[.75, .25])
sgd.fit(X[train], y[train])

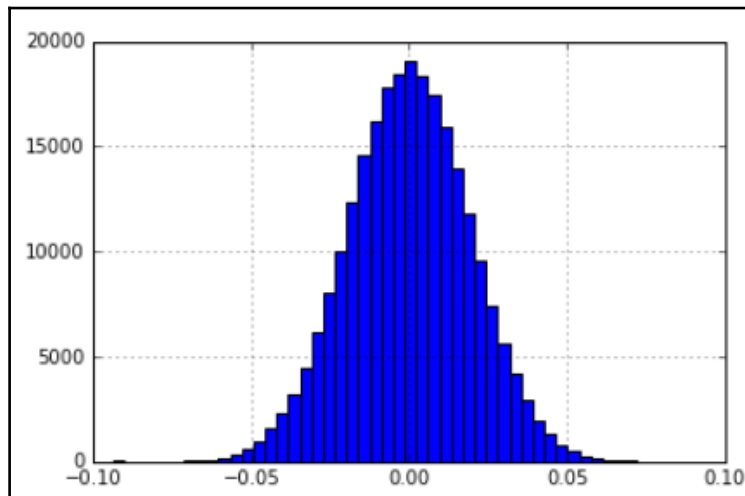
SGDRegressor(alpha=0.0001, average=False, epsilon=0.1, eta0=0.01,
             fit_intercept=True, l1_ratio=0.15,
```

```
learning_rate='invscaling',  
    loss='squared_loss', n_iter=5, penalty='l2', power_t=0.25,  
    random_state=None, shuffle=True, verbose=0,  
    warm_start=False)
```

So, we have another beefy object. The main thing to know now is that our loss function is `squared_loss`, which is the same thing that occurs during linear regression. It is also worth noting that `shuffle` will generate a random shuffle of the data. This is useful if you want to break a potentially spurious correlation. With `x`, scikit-learn will automatically include a column of ones.

6. We can then predict, as we previously have, using scikit-learn's consistent API. You can see we actually got a really good fit. There is barely any variation, and the histogram has a nice normal look.:

```
y_pred = sgd.predict(X[~train])  
  
%matplotlib inline  
import pandas as pd  
  
pd.Series(y[~train] - y_pred).hist(bins=50)
```



How it works...

Clearly, the fake dataset we used wasn't too bad, but you can imagine datasets with larger magnitudes. For example, if you worked on Wall Street on any given day, there might be 2 billion transactions on any given exchange in a market. Now, imagine that you have a week's or a year's data. Running in-core algorithms does not work with huge volumes of data.

The reason this is normally difficult is that to do SGD, we're required to calculate the gradient at every step. The gradient has the standard definition from any third calculus course.

The gist of the algorithm is that at each step, we calculate a new set of coefficients and update this with a learning rate and the outcome of the objective function. In pseudocode, this might look like the following:

```
while not converged:
    w = w - learning_rate*gradient(cost(w))
```

The relevant variables are as follows:

- `w`: This is the coefficient matrix.
- `learning_rate`: This shows how big a step to take at each iteration. This might be important to tune if you aren't getting good convergence.
- `gradient`: This is the matrix of second derivatives.
- `cost`: This is the squared error for regression. We'll see later that this cost function can be adapted to work with classification tasks. This flexibility is one thing that makes SGD so useful.

This will not be so bad, except for the fact that the gradient function is expensive. As the vector of coefficients gets larger, calculating the gradient becomes very expensive. For each update step, we need to calculate a new weight for every point in the data, and then update. SGD works slightly differently; instead of the previous definition for batch gradient descent, we'll update the parameter with each new data point. This data point is picked at random, hence the name stochastic gradient descent.

A final note on SGD is that it is a meta-heuristic that gives a lot of power to several machine learning algorithms. It is worth checking out some papers on meta-heuristics applied to various machine learning algorithms. Cutting-edge solutions might be innocently hidden in such papers.

3

Dimensionality Reduction

In this chapter, we will cover the following recipes:

- Reducing dimensionality with PCA
- Using factor analysis for decomposition
- Using kernel PCA for nonlinear dimensionality reduction
- Using truncated SVD to reduce dimensionality
- Using decomposition to classify with DictionaryLearning
- Doing dimensionality reduction with manifolds – t-SNE
- Testing methods to reduce dimensionality with pipelines

Introduction

In this chapter, we will reduce the number of features or inputs into the machine learning models. This is a very important operation because sometimes datasets have a lot of input columns, and reducing the number of columns creates simpler models that take less computing power to predict.

The main model used in this section is **principal component analysis (PCA)**. You do not have to know how many features you can reduce the dataset to, thanks to PCA's explained variance. A similar model in performance is **truncated singular value decomposition (truncated SVD)**. It is always best to first choose a linear model that allows you to know how many columns you can reduce the set to, such as PCA or truncated SVD.

Later in the chapter, check out the modern method of **t-distributed stochastic neighbor embedding (t-SNE)**, which makes features easier to visualize in lower dimensions. In the final recipe, you can examine a complex pipeline and grid search that finds the best composite estimator consisting of dimensionality reductions joined with several support vector machines.

Reducing dimensionality with PCA

Now it's time to take the math up a level! PCA is the first somewhat advanced technique discussed in this book. While everything else thus far has been simple statistics, PCA will combine statistics and linear algebra to produce a preprocessing step that can help to reduce dimensionality, which can be the enemy of a simple model.

Getting ready

PCA is a member of the decomposition module of scikit-learn. There are several other decomposition methods available, which will be covered later in this recipe. Let's use the iris dataset, but it's better if you use your own data:

```
from sklearn import datasets
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
%matplotlib inline

iris = datasets.load_iris()
iris_X = iris.data
y = iris.target
```

How to do it...

1. Import the `decomposition` module:

```
from sklearn import decomposition
```

2. Instantiate a default PCA object:

```
pca = decomposition.PCA()
pca
```

```
PCA(copy=True, iterated_power='auto', n_components=None,
    random_state=None,
    svd_solver='auto', tol=0.0, whiten=False)
```

3. Compared to other objects in scikit-learn, the PCA object takes relatively few arguments. Now that the PCA object (an instance PCA) has been created, simply transform the data by calling the `fit_transform` method, with `iris_X` as the argument:

```
iris_pca = pca.fit_transform(iris_X)
iris_pca[:5]

array([[ -2.68420713e+00,   3.26607315e-01,  -2.15118370e-02,
         1.00615724e-03],
       [ -2.71539062e+00,  -1.69556848e-01,  -2.03521425e-01,
         9.96024240e-02],
       [ -2.88981954e+00,  -1.37345610e-01,   2.47092410e-02,
         1.93045428e-02],
       [ -2.74643720e+00,  -3.11124316e-01,   3.76719753e-02,
        -7.59552741e-02],
       [ -2.72859298e+00,   3.33924564e-01,   9.62296998e-02,
        -6.31287327e-02]])
```

4. Now that the PCA object has been fitted, we can see how well it has done at explaining the variance (explained in the following *How it works...* section):

```
pca.explained_variance_ratio_
array([ 0.92461621,  0.05301557,  0.01718514,  0.00518309])
```

How it works...

PCA has a general mathematical definition and a specific use case in data analysis. PCA finds the set of orthogonal directions that represent the original data matrix.

Generally, PCA works by mapping the original dataset into a new space where each of the new column vectors of the matrix are orthogonal. From a data analysis perspective, PCA transforms the covariance matrix of the data into column vectors that can explain certain percentages of the variance. For example, with the iris dataset, 92.5 percent of the variance of the overall dataset can be explained by the first component.

This is extremely useful because dimensionality is problematic in data analysis. Quite often, algorithms applied to high-dimensional datasets will overfit on the initial training, and thus lose generality to the test set. If most of the underlying structure of the data can be faithfully represented by fewer dimensions, then it's generally considered a worthwhile trade-off:

```
pca = decomposition.PCA(n_components=2)
iris_X_prime = pca.fit_transform(iris_X)
iris_X_prime.shape
(150L, 2L)
```

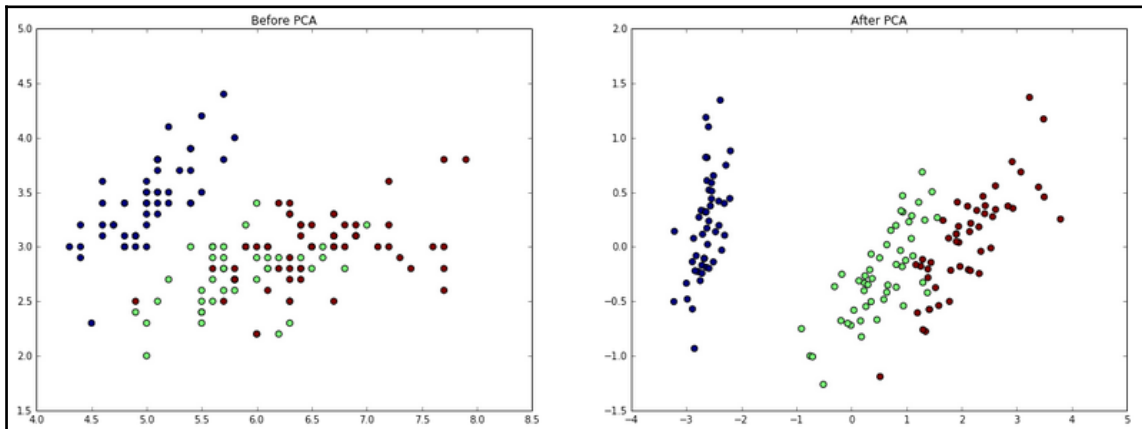
Our data matrix is now 150×2 , instead of 150×4 . The separability of the classes remains even after reducing the dimensionality by two. We can see how much of the variance is represented by the two components that remain:

```
pca.explained_variance_ratio_.sum()
0.97763177502480336
```

To visualize what PCA has done, let's plot the first two dimensions of the iris dataset with before-after pictures of the PCA transformation:

```
fig = plt.figure(figsize=(20, 7))
ax = fig.add_subplot(121)
ax.scatter(iris_X[:, 0], iris_X[:, 1], c=y, s=40)
ax.set_title('Before PCA')

ax2 = fig.add_subplot(122)
ax2.scatter(iris_X_prime[:, 0], iris_X_prime[:, 1], c=y, s=40)
ax2.set_title('After PCA')
```



The PCA object can also be created with the amount of explained variance in mind from the start. For example, if we want to be able to explain at least 98 percent of the variance, the PCA object will be created as follows:

```
pca = decomposition.PCA(n_components=.98)
iris_X_prime = pca.fit(iris_X).transform(iris_X)
pca.explained_variance_ratio_.sum()
0.99481691454981014
```

Since we wanted to explain variance slightly more than the two component examples, a third was included.



Even though the final dimensions of the data are two or three, these two or three columns contain information from all four original columns.

There's more...

It is recommended that PCA is scaled beforehand. Do so as follows:

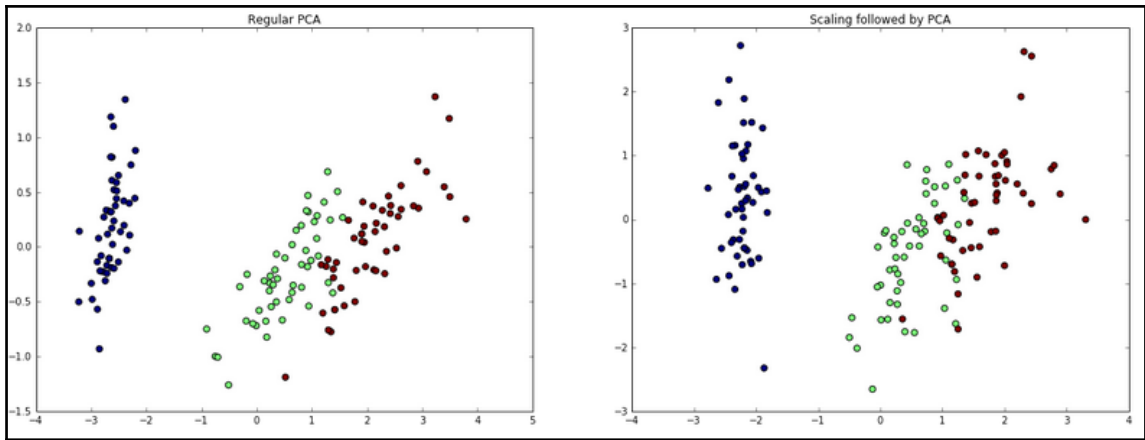
```
from sklearn import preprocessing

iris_X_scaled = preprocessing.scale(iris_X)
pca = decomposition.PCA(n_components=2)
iris_X_scaled = pca.fit_transform(iris_X_scaled)
```

This leads to the following graph:

```
fig = plt.figure(figsize=(20,7))
ax = fig.add_subplot(121)
ax.scatter(iris_X_prime[:,0],iris_X_prime[:,1],c=y,s=40)
ax.set_title('Regular PCA')

ax2 = fig.add_subplot(122)
ax2.scatter(iris_X_scaled[:,0],iris_X_scaled[:,1],c=y,s=40)
ax2.set_title('Scaling followed by PCA')
```



This looks a bit worse. Regardless, you should always consider the scaled PCA if you consider PCA. Preferably, you can scale with a pipeline as follows:

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

pipe = Pipeline([('scaler', StandardScaler()),
                  ('pca', decomposition.PCA(n_components=2))])
iris_X_scaled = pipe.fit_transform(iris_X)
```

Using pipelines prevents errors and reduces the amount of debugging of complex code.

Using factor analysis for decomposition

Factor analysis is another technique that we can use to reduce dimensionality. However, factor analysis makes assumptions and PCA does not. The basic assumption is that there are implicit features responsible for the features of the dataset.

This recipe will boil down to the explicit features from our samples in an attempt to understand the independent variables as much as the dependent variables.

Getting ready

To compare PCA and factor analysis, let's use the iris dataset again, but we'll first need to load the `FactorAnalysis` class:

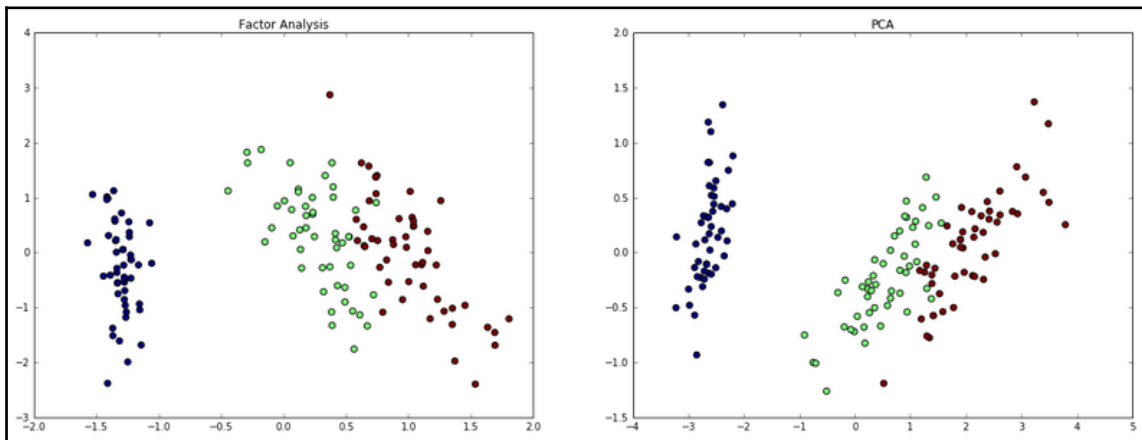
```
from sklearn import datasets
iris = datasets.load_iris()
iris_X = iris.data
from sklearn.decomposition import FactorAnalysis
```

How to do it...

From a programming perspective, factor analysis isn't much different from PCA:

```
fa = FactorAnalysis(n_components=2)
iris_two_dim = fa.fit_transform(iris.data)
iris_two_dim[:5]
array([[ -1.33125848, -0.55846779],
       [ -1.33914102,  0.00509715],
       [ -1.40258715,  0.307983  ],
       [ -1.29839497,  0.71854288],
       [ -1.33587575, -0.36533259]])
```

Compare the following plot to the plot in the last section:



Since factor analysis is a probabilistic transform, we can examine different aspects, such as the log likelihood of the observations under the model, and better still, compare the log likelihoods across models.

Factor analysis is not without flaws. The reason is that you're not fitting a model to predict an outcome, you're fitting a model as a preparation step. This isn't a bad thing, but errors here are compounded when training the actual model.

How it works...

Factor analysis is similar to PCA, which was covered previously. However, there is an important distinction to be made. PCA is a linear transformation of the data to a different space where the first component explains the variance of the data, and each subsequent component is orthogonal to the first component.

For example, you can think of PCA as taking a dataset of N dimensions and going down to some space of M dimensions, where $M < N$.

Factor analysis, on the other hand, works under the assumption that there are only M important features and a linear combination of these features (plus noise) creates the dataset in N dimensions. To put it another way, you don't do regression on an outcome variable, you do regression on the features to determine the latent factors of the dataset.

Additionally, a big drawback is that you do not know how many columns you can reduce the data to. PCA gives you the explained variance metric to guide you through the process.

Using kernel PCA for nonlinear dimensionality reduction

Most of the techniques in statistics are linear by nature, so in order to capture nonlinearity, we might need to apply some transformation. PCA is, of course, a linear transformation. In this recipe, we'll look at applying nonlinear transformations, and then apply PCA for dimensionality reduction.

Getting ready

Life would be so easy if data was always linearly separable, but unfortunately, it's not. Kernel PCA can help to circumvent this issue. Data is first run through the kernel function that projects the data onto a different space; then, PCA is performed.

To familiarize yourself with the kernel functions, it will be a good exercise to think of how to generate data that is separable by the kernel functions available in the kernel PCA. Here, we'll do that with the cosine kernel. This recipe will have a bit more theory than the previous recipes.

Before starting, load the iris dataset:

```
from sklearn import datasets, decomposition
iris = datasets.load_iris()
iris_X = iris.data
```

How to do it...

The cosine kernel works by comparing the angle between two samples represented in the feature space. It is useful when the magnitude of the vector perturbs the typical distance measure used to compare samples. As a reminder, the cosine between two vectors is given by the following formula:

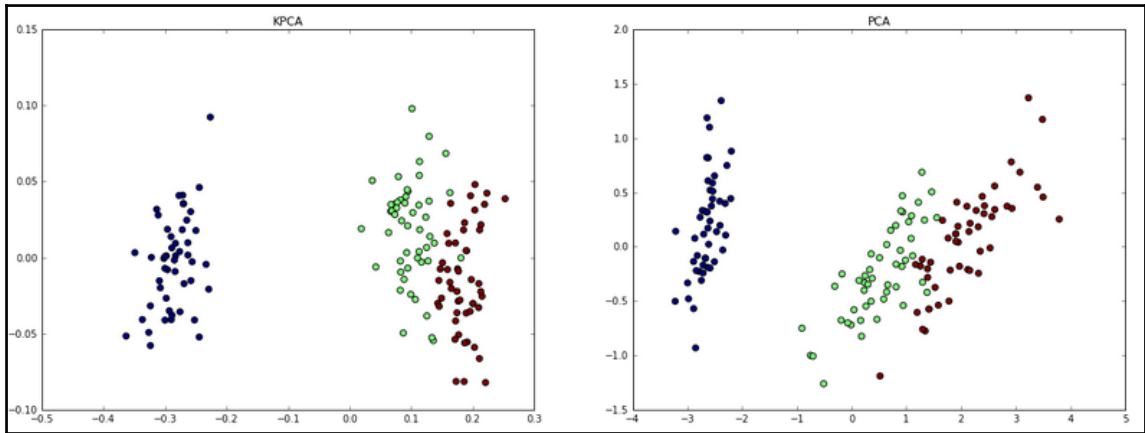
$$\cos(\theta) = \frac{A \cdot B}{\|A\| \|B\|}$$

This means that the cosine between A and B is the dot product of the two vectors normalized by the product of the individual norms. The magnitude of vectors A and B have no influence on this calculation.

So, let's go back to the iris dataset to use it for visual comparisons:

```
kpca = decomposition.KernelPCA(kernel='cosine', n_components=2)
iris_X_prime = kpca.fit_transform(iris_X)
```

Then, visualize the result:



The result looks slightly better, although we would have to measure it to know for sure.

How it works...

There are several different kernels available besides the cosine kernel. You can even write your own kernel function. The available kernels are as follows:

- Poly (polynomial)
- RBF (radial basis function)
- Sigmoid
- Cosine
- Pre-computed

There are also options that are contingent on the kernel choice. For example, the degree argument will specify the degree for the poly, RBF, and sigmoid kernels; also, gamma will affect the RBF or poly kernels.

The recipe on SVM will cover the RBF kernel function in more detail.



Kernel methods are great to create separability, but they can also cause overfitting if used without care. Make sure to train-test them properly.

Luckily, the available kernels are smooth, continuous, and differentiable functions. They do not create the jagged edges of regression trees.

Using truncated SVD to reduce dimensionality

Truncated SVD is a matrix factorization technique that factors a matrix M into the three matrices U , Σ , and V . This is very similar to PCA, except that the factorization for SVD is done on the data matrix, whereas for PCA, the factorization is done on the covariance matrix. Typically, SVD is used under the hood to find the principle components of a matrix.

Getting ready

Truncated SVD is different from regular SVDs in that it produces a factorization where the number of columns is equal to the specified truncation. For example, given an $n \times n$ matrix, SVD will produce matrices with n columns, whereas truncated SVD will produce matrices with the specified number of columns. This is how the dimensionality is reduced. Here, we'll again use the iris dataset so that you can compare this outcome against the PCA outcome:

```
from sklearn.datasets import load_iris
iris = load_iris()
iris_X = iris.data
y = iris.target
```

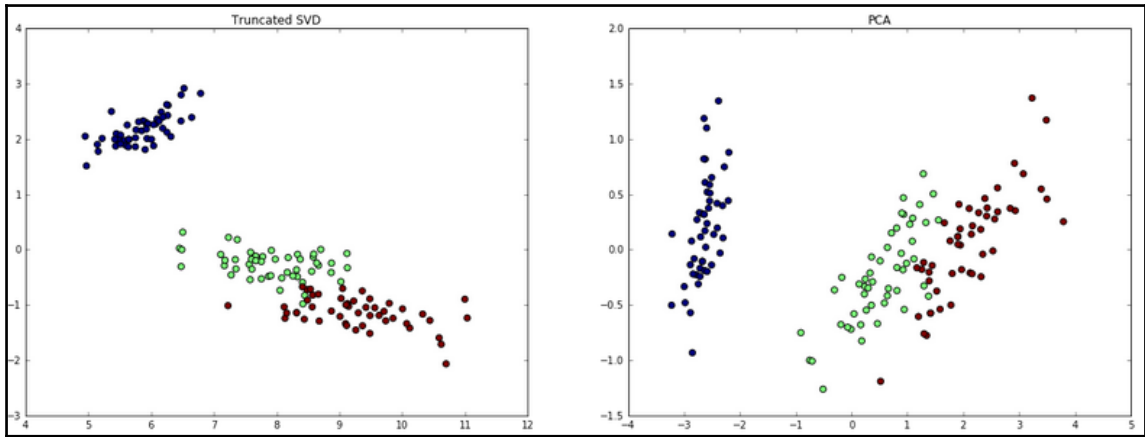
How to do it...

This object follows the same form as the other objects we've used.

First, we'll import the required object, then we'll fit the model and examine the results:

```
from sklearn.decomposition import TruncatedSVD
svd = TruncatedSVD(2)
iris_transformed = svd.fit_transform(iris_X)
```


Then, visualize the results:



The results look pretty good. Like PCA, there is explained variance with `explained_variance_ratio_`:

```
svd.explained_variance_ratio_  
array([ 0.53028106,  0.44685765])
```

How it works...

Now that we've walked through how, is performed in scikit-learn, let's look at how we can use only SciPy, and learn a bit in the process.

First, we need to use SciPy's `linalg` to perform SVD:

```
from scipy.linalg import svd  
import numpy as np  
D = np.array([[1, 2], [1, 3], [1, 4]])  
D  
  
array([[1, 2],  
       [1, 3],  
       [1, 4]])  
  
U, S, V = svd(D, full_matrices=False)  
  
U.shape, S.shape, V.shape  
((3L, 2L), (2L,), (2L, 2L))
```

We can reconstruct the original matrix D to confirm U , S , and V as a decomposition:

```
np.dot(U.dot(np.diag(S)), V)

array([[1, 2],
       [1, 3],
       [1, 4]])
```

The matrix that is actually returned by truncated SVD is the dot product of the U and S matrices. If we want to simulate the truncation, we will drop the smallest singular values and the corresponding column vectors of U . So, if we want a single component here, we do the following:

```
new_S = S[0]
new_U = U[:, 0]
new_U.dot(new_S)

array([-2.20719466, -3.16170819, -4.11622173])
```

In general, if we want to truncate to some dimensionality, for example, t , we drop $N - t$ singular values.

There's more...

Truncated SVD has a few miscellaneous things that are worth noting with respect to the method.

Sign flipping

There's a gotcha with truncated SVDs. Depending on the state of the random number generator, successive fittings of truncated SVD can flip the signs of the output. In order to avoid this, it's advisable to fit truncated SVD once, and then use transforms from then on. This is another good reason for pipelines!

To carry this out, do the following:

```
tsvd = TruncatedSVD(2)
tsvd.fit(iris_X)
tsvd.transform(iris_X)
```

Sparse matrices

One advantage of truncated SVD over PCA is that truncated SVD can operate on sparse matrices, while PCA cannot. This is due to the fact that the covariance matrix must be computed for PCA, which requires operating on the entire matrix.

Using decomposition to classify with DictionaryLearning

In this recipe, we'll show how a decomposition method can actually be used for classification. `DictionaryLearning` attempts to take a dataset and transform it into a sparse representation.

Getting ready

With `DictionaryLearning`, the idea is that the features are the basis for the resulting datasets. Load the iris dataset:

```
from sklearn.datasets import load_iris
iris = load_iris()
iris_X = iris.data
y = iris.target
```

Additionally, create a training set by taking every other element of `iris_X` and `y`. Take the remaining elements for testing:

```
X_train = iris_X[::2]
X_test = iris_X[1::2]
y_train = y[::2]
y_test = y[1::2]
```

How to do it...

1. Import `DictionaryLearning`:

```
from sklearn.decomposition import DictionaryLearning
```

2. Use three components to represent the three species of iris:

```
dl = DictionaryLearning(3)
```

3. Transform every other data point so that we can test the classifier on the resulting data points after the learner is trained:

```
transformed = dl.fit_transform(X_train)
transformed[:5]

array([[ 0.          ,  6.34476574,  0.          ],
       [ 0.          ,  5.83576461,  0.          ],
       [ 0.          ,  6.32038375,  0.          ],
       [ 0.          ,  5.89318572,  0.          ],
       [ 0.          ,  5.45222715,  0.          ]])
```

4. Now test the transform simply by typing the following:

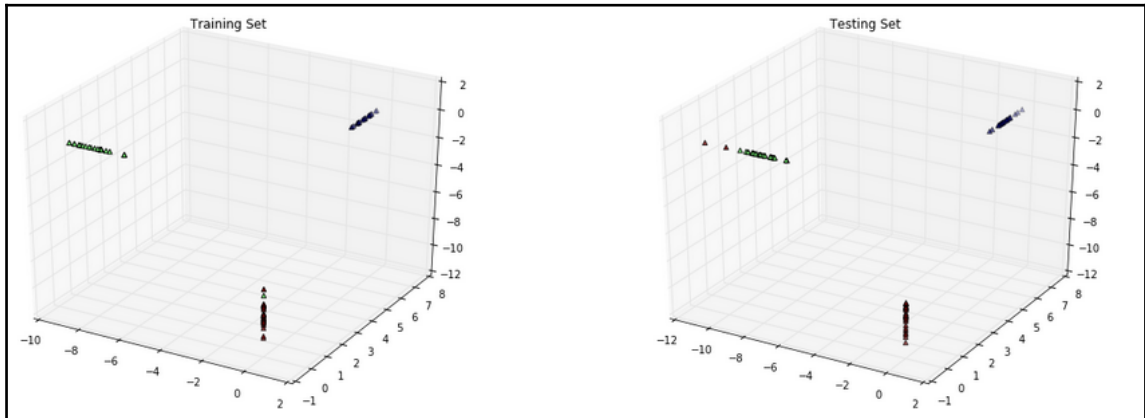
```
test_transform = dl.transform(X_test)
```

We can visualize the output. Notice how each value is sited on the x , y , or z axis, along with the other values and zero; this is called sparseness:

```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt

fig = plt.figure(figsize=(14,7))
ax = fig.add_subplot(121, projection='3d')
ax.scatter(transformed[:,0],transformed[:,1],transformed[:,2],c=y_train,marker = '^')
ax.set_title("Training Set")
```

```
ax2 = fig.add_subplot(122, projection='3d')
ax2.scatter(test_transform[:,0],test_transform[:,1],test_transform[:,2],c=y_
_test,marker = '^')
ax2.set_title("Testing Set")
```



If you look closely, you can see there was a training error. One of the classes was misclassified. Only being wrong once isn't a big deal, though. There was also an error in the classification. If you remember some of the other visualizations, the red and green classes were the two classes that often appeared close together.

How it works...

DictionaryLearning has a background in signal processing and neurology. The idea is that only few features can be active at any given time. Therefore, `DictionaryLearning` attempts to find a suitable representation of the underlying data, given the constraint that most of the features should be zero.

Doing dimensionality reduction with manifolds – t-SNE

Getting ready

This is a short and practical recipe.

If you read the rest of the chapter, we have been doing a lot of dimensionality reduction with the iris dataset. Let's continue the pattern for additional easy comparisons. Load the iris dataset:

```
from sklearn.datasets import load_iris
iris = load_iris()
iris_X = iris.data
y = iris.target
```

Load PCA and some classes from the manifold module:

```
from sklearn.decomposition import PCA
from sklearn.manifold import TSNE, MDS, Isomap

#Load visualization library
import matplotlib.pyplot as plt
%matplotlib inline
```

How to do it...

1. Run all the transforms on `iris_X`. One of the transforms is t-SNE:

```
iris_pca = PCA(n_components = 2).fit_transform(iris_X)
iris_tsne = TSNE(learning_rate=200).fit_transform(iris_X)

iris_MDS = MDS(n_components = 2).fit_transform(iris_X)
iris_ISO = Isomap(n_components = 2).fit_transform(iris_X)
```

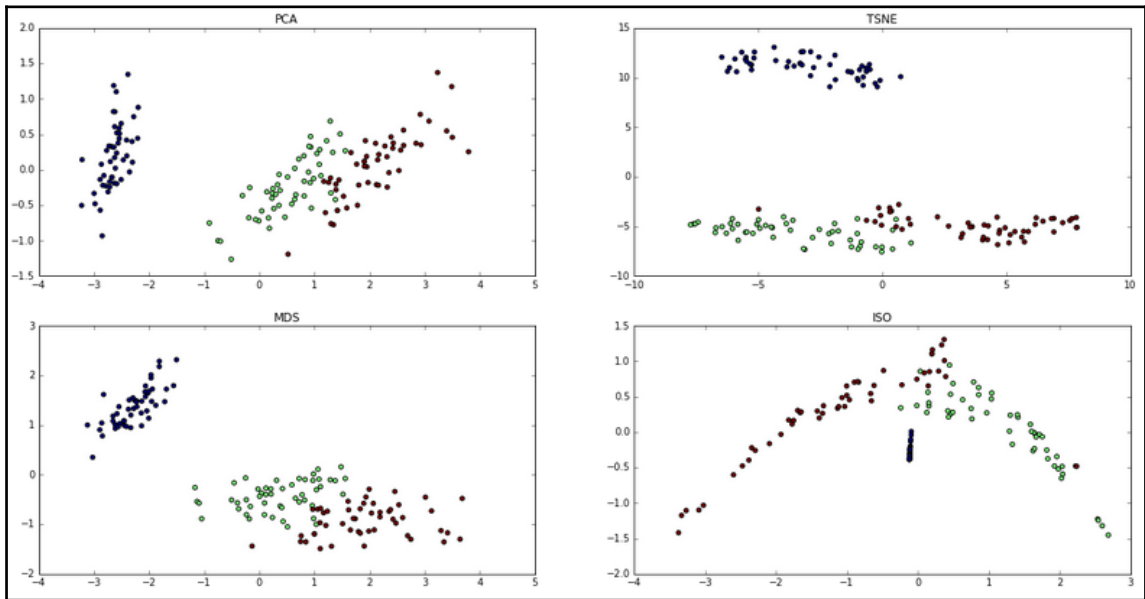
2. Plot the results:

```
plt.figure(figsize=(20, 10))
plt.subplot(221)
plt.title('PCA')
plt.scatter(iris_pca[:, 0], iris_pca[:, 1], c=y)
```

```
plt.subplot(222)
plt.scatter(iris_tsne[:, 0], iris_tsne[:, 1], c=y)
plt.title('TSNE')

plt.subplot(223)
plt.scatter(iris_MDS[:, 0], iris_MDS[:, 1], c=y)
plt.title('MDS')

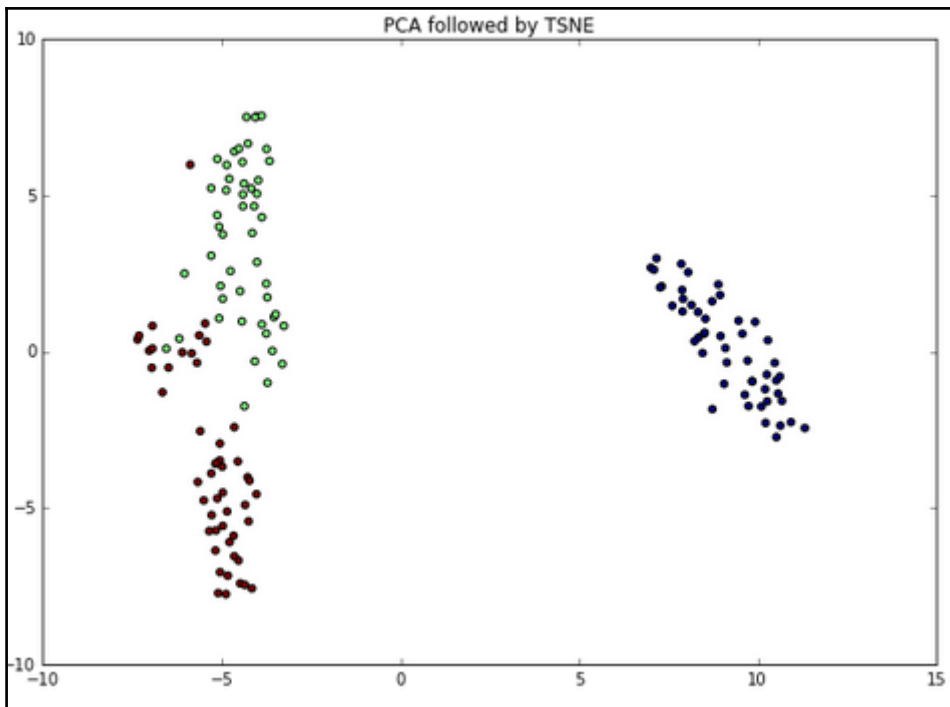
plt.subplot(224)
plt.scatter(iris_ISO[:, 0], iris_ISO[:, 1], c=y)
plt.title('ISO')
```



The t-SNE algorithm has been popular recently, yet it takes a lot of computing time and power. ISO produces an interesting graphic.

Additionally, in cases where the dimensionality of the data is very high (more than 50 columns) the scikit-learn documentation suggests doing PCA or truncated SVD before t-SNE. The iris dataset is small, but we can write the syntax to perform t-SNE after PCA:

```
iris_pca_then_tsne = TSNE(learning_rate=200).fit_transform(iris_pca)
plt.figure(figsize=(10, 7))
plt.scatter(iris_pca_then_tsne[:, 0], iris_pca_then_tsne[:, 1], c=y)
plt.title("PCA followed by TSNE")
```



How it works...

In mathematics, a manifold is a space that is locally Euclidean at every point, yet is embedded in a higher-dimensional space. For example, the outer surface of a sphere is a two-dimensional manifold in three dimensions. When we walk around on the surface of the sphere of the Earth, we tend to perceive the 2D plane of the ground rather than all of 3D space. We navigate using 2D maps, not higher-dimensional ones.

The `manifold` module in `scikit-learn` is useful for understanding high-dimensional spaces in two or three dimensions. The algorithms in the module gather information about the local structure around a point and seek to preserve it. What are the neighbors of a point? How far away are the neighbors of a point?

For example, the Isomap algorithm attempts to preserve geodesic distances between all of the points in an algorithm, starting with a nearest neighbor search, followed by a graph search, and then a partial eigenvalue decomposition. The point of the algorithm is to preserve distances and a manifold's local geometric structure. The **multi-dimensional scaling (MDS)** algorithm also respects distances.

t-SNE converts Euclidean distances between pairs of points in the dataset into probabilities. Around each point there is a Gaussian centered at that point, and the probability distribution represents the chance of any other point being a neighbor. Points very far away from each other have a low chance of being neighbors. Here, we have turned point locations into distances and then probabilities. t-SNE maintains the local structure very well by utilizing the probabilities of two points being neighbors.

In a very general sense manifold methods start by examining the neighbors of every point, which represent the local structure of a manifold, and attempt to preserve that local structure in different ways. It is similar to you walking around your neighborhood or block constructing a 2D map of the local structure around you and focusing on two dimensions rather than three.

Testing methods to reduce dimensionality with pipelines

Here we will see how different estimators composed of dimensionality reduction and a support vector machine perform.

Getting ready

Load the iris dataset and some dimensionality reduction libraries. This is a big step for this particular recipe:

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.datasets import load_iris
from sklearn.model_selection import GridSearchCV
from sklearn.pipeline import Pipeline
from sklearn.svm import SVC, LinearSVC
from sklearn.decomposition import PCA, NMF, TruncatedSVD
from sklearn.manifold import Isomap
%matplotlib inline
```

How to do it...

1. Instantiate a pipeline object with two main parts:
 - An object to reduce dimensionality
 - An estimator with a predict method

```
pipe = Pipeline([
    ('reduce_dim', PCA()),
    ('classify', SVC())
])
```

2. Note in the following code that Isomap comes from the `manifold` module and that the **non-negative matrix factorization** (NMF) algorithm utilizes SVDs to break up a matrix into non-negative factors, its main purpose in this section is to compare its performance with other algorithms, but it is useful in **natural language processing** (NLP) where matrix factorizations cannot be negative. Now type the following parameter grid:

```
param_grid = [
    {
        'reduce_dim': [PCA(), NMF(), Isomap(), TruncatedSVD()],
        'reduce_dim__n_components': [2, 3],
        'classify' : [SVC(), LinearSVC()],
        'classify__C': [1, 10, 100, 1000]
    },
]
```

This parameter grid will allow scikit-learn to cycle through a few dimensionality reduction techniques coupled with two SVM types: linear SVC and SVC for classification.

3. Now run a grid search:

```
grid = GridSearchCV(pipe, cv=3, n_jobs=-1, param_grid=param_grid)
iris = load_iris()
grid.fit(iris.data, iris.target)
```

4. Now look at the best parameters to determine the best model. A PCA with SVC was the best model:

```
grid.best_params_

{'classify': SVC(C=10, cache_size=200, class_weight=None,
coef0=0.0,
    decision_function_shape=None, degree=3, gamma='auto',
kernel='rbf',
    max_iter=-1, probability=False, random_state=None,
shrinking=True,
    tol=0.001, verbose=False),
'classify__C': 10,
'reduce_dim': PCA(copy=True, iterated_power='auto',
n_components=3, random_state=None,
    svd_solver='auto', tol=0.0, whiten=False),
'reduce_dim__n_components': 3}

grid.best_score_

0.97999999999999998
```

5. If you would like to create a dataframe of results, use the following command:

```
import pandas as pd
results_df = pd.DataFrame(grid.cv_results_)
```

6. Finally, you can predict on an unseen instance with the `grid.predict(X_test)` method for a testing set `X_test`. We will do several grid searches in later chapters.

How it works...

Grid search does cross-validation to determine the best score. In this case, all the data was used for three-fold cross-validation. For the rest of the book, we will save some data for testing to make sure the models do not run into anomalous behavior.

A final note on the pipeline you just saw: the `sklearn.decomposition` methods will work for the first step of reducing dimensionality within the pipeline, but not all of the manifold methods were designed for pipelines.

4

Linear Models with scikit-learn

This chapter contains the following recipes:

- Fitting a line through data
- Fitting a line through data with machine learning
- Evaluating the linear regression model
- Using ridge regression to overcome linear regression's shortfalls
- Optimizing the ridge regression parameter
- Using sparsity to regularize models
- Taking a more fundamental approach to regularization with LARS

Introduction

I conjecture that we are built to perceive linear functions very well. They are very easy to visualize, interpret, and explain. Linear regression is very old and was probably the first statistical model.

In this chapter, we will take a machine learning approach to linear regression.

Note that this chapter, similar to the chapter on dimensionality reduction and PCA, involves selecting the best features using linear models. Even if you decide not to perform regression for predictions with linear models, you can select the most powerful features.

Also note that linear models provide a lot of the intuition behind the use of many machine learning algorithms. For example, RBF-kernel SVMs have smooth boundaries, which when looked at up close, look like a line. Thus, SVMs are often easy to explain if, in the background, you remember your linear model intuition.

Fitting a line through data

Now we will start with some basic modeling with linear regression. Traditional linear regression is the first, and therefore, probably the most fundamental model—a straight line through data.

Intuitively, it is familiar to a lot of the population: a change in one input variable proportionally changes the output variable. It is important that many people will have seen it in school, or in a newspaper data graphic, or in a presentation at work, and so on, as it will be easy for you to explain to colleagues and investors.

Getting ready

The Boston dataset is perfect to play around with regression. The Boston dataset has the median home price of several areas in Boston. It also has other factors that might impact housing prices, for example, crime rate. First, import the `datasets` model, then we can load the dataset:

```
from sklearn import datasets
boston = datasets.load_boston()
```

How to do it...

Actually, using linear regression in scikit-learn is quite simple. The API for linear regression is basically the same API you're now familiar with from the previous chapter.

1. First, import the `LinearRegression` object and create an object:

```
from sklearn.linear_model import LinearRegression
lr = LinearRegression()
```

2. Now, it's as easy as passing the independent and dependent variables to the `fit` method of `LinearRegression`:

```
lr.fit(boston.data, boston.target)
LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1,
normalize=False)
```

3. Now, to get the predictions, do the following:

```
predictions = lr.predict(boston.data)
```

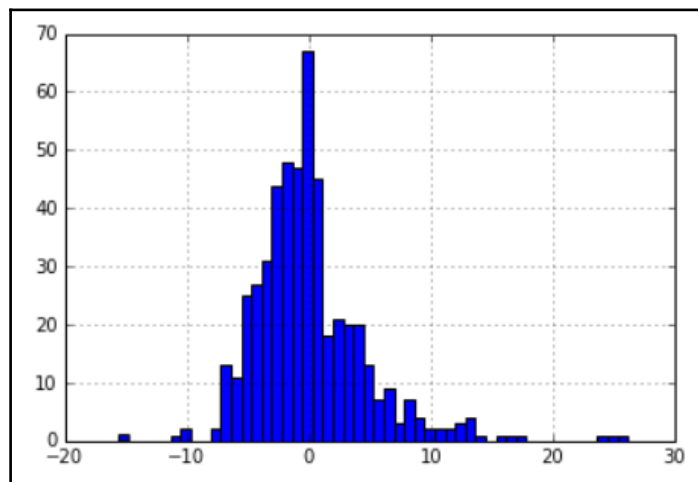
4. You have obtained the predictions produced by linear regression. Now, explore the `LinearRegression` class a bit more. Look at the residuals, the difference between the real target set and the predicted target set:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

#within an Ipython notebook:

%matplotlib inline

pd.Series(boston.target - predictions).hist(bins=50)
```



A common pattern to express the coefficients of features and their names is `zip(boston.feature_names, lr.coef_)`.

5. Find the coefficients of the linear regression by typing `lr.coef_`:

```
lr.coef_
array([ -1.07170557e-01,   4.63952195e-02,   2.08602395e-02,
         2.68856140e+00,  -1.77957587e+01,   3.80475246e+00,
```

```

7.51061703e-04, -1.47575880e+00, 3.05655038e-01,
-1.23293463e-02, -9.53463555e-01, 9.39251272e-03,
-5.25466633e-01])

```

So, going back to the data, we can see which factors have a negative relationship with the outcome, and also the factors that have a positive relationship. For example, and as expected, an increase in the per capita crime rate by town has a negative relationship with the price of a home in Boston. The per capita crime rate is the first coefficient in the regression.

6. You can also look at the intercept, the predicted value of the target, when all input variables are zero:

```

lr.intercept_

36.491103280361955

```

7. If you forget the names of the coefficients or intercept attributes, type `dir(lr)`:

```

[... #partial output due to length
'coef_',
'copy_X',
'decision_function',
'fit',
'fit_intercept',
'get_params',
'intercept_',
'n_jobs',
'normalize',
'predict',
'rank_',
'residues_',
'score',
'set_params',
'singular_']

```

For many scikit-learn predictors, parameters that consist of a word followed by a single `_` such as `coef_` or `intercept_`, are of special interest. Using the `dir` command is a good way to check what is available within the scikit predictor implementation.

How it works...

The basic idea of linear regression is to find the set of coefficients of v that satisfy $y = Xv$, where X is the data matrix. It's unlikely that, for the given values of X , we will find a set of coefficients that exactly satisfy the equation; an error term gets added if there is an inexact specification or measurement error.

Therefore, the equation becomes $y = Xv + e$, where e is assumed to be normally distributed and independent of the X values. Geometrically, this means that the error terms are perpendicular to X . This is beyond the scope of this book, but it might be worth proving $E(Xv) = 0$ for yourself.

There's more...

The `LinearRegression` object can automatically normalize (or scale) inputs:

```
lr2 = LinearRegression(normalize=True)
lr2.fit(boston.data, boston.target)
LinearRegression(copy_X=True, fit_intercept=True, normalize=True)
predictions2 = lr2.predict(boston.data)
```

Fitting a line through data with machine learning

Linear regression with machine learning involves testing the linear regression algorithm on unseen data. Here, we will perform 10-fold cross-validation:

- Split the set into 10 parts
- Train on 9 of the parts and test on the one left over
- Repeat this 10 times so that every part gets to be a test set once

Getting ready

As in the previous section, load the dataset you want to apply linear regression to, in this case, the Boston housing dataset:

```
from sklearn import datasets
boston = datasets.load_boston()
```


How to do it...

The steps involved in performing linear regression are as follows:

1. Import the `LinearRegression` object and create an object:

```
from sklearn.linear_model import LinearRegression
lr = LinearRegression()
```

2. Pass the independent and dependent variables to the `fit` method of `LinearRegression`:

```
lr.fit(boston.data, boston.target)

LinearRegression(copy_X=True, fit_intercept=True, n_jobs=1,
normalize=False)
```

3. Now, to get the 10-fold cross-validated predictions, do the following:

```
from sklearn.model_selection import cross_val_predict

predictions_cv = cross_val_predict(lr, boston.data, boston.target,
cv=10)
```

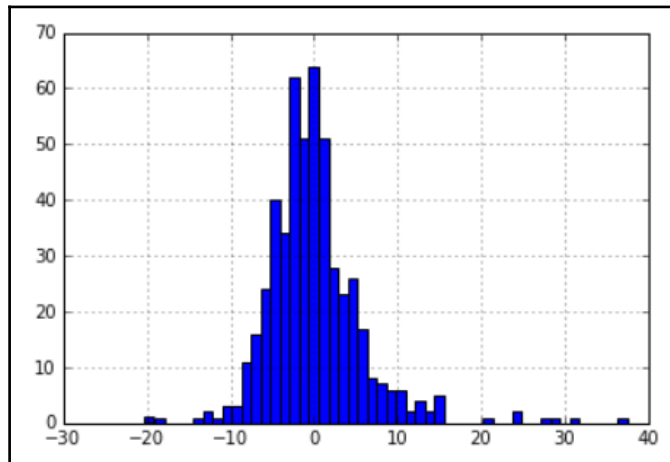
4. Looking at the residuals, the difference between the real data and the predictions, they are more normally distributed compared to the residuals in the previous section of linear regression without cross-validation:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

#within Ipython
%matplotlib inline

pd.Series(boston.target - predictions_cv).hist(bins=50)
```

5. The following are the new residuals through cross-validation. The normal distribution is more symmetric than it was previously without cross-validation:



Evaluating the linear regression model

In this recipe, we'll look at how well our regression fits the underlying data. We fitted a regression in the last recipe, but didn't pay much attention to how well we actually did it. The first question after we fitted the model was clearly, how well does the model fit? In this recipe, we'll examine this question.

Getting ready

Let's use the `lr` object and Boston dataset—reach back into your code from the *Fitting a line through data* recipe. The `lr` object will have a lot of useful methods now that the model has been fit.

How to do it...

1. Start within IPython with several imports, including `numpy`, `pandas`, and `matplotlib` for visualization:

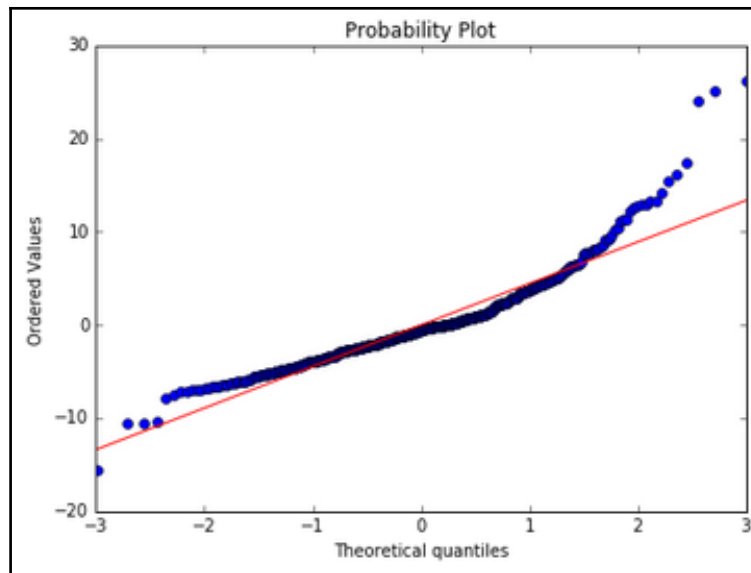
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
```

```
%matplotlib inline
```

2. It is worth looking at a Q-Q plot. We'll use `scipy` here because it has a built-in probability plot:

```
from scipy.stats import probplot
f = plt.figure(figsize=(7, 5))
ax = f.add_subplot(111)
tuple_out = probplot(boston.target - predictions_cv, plot=ax)
```

The following screenshot shows the probability plot:



3. Type `tuple_out[1]` and you will get the following:

```
(4.4568597454452306, -2.9208080837569337e-15, 0.94762914118318298)
```

This is a tuple of the form (*slope*, *intercept*, *r*), where *slope* and *intercept* come from the least-squares fit and *r* is the square root of the coefficient of determination.

4. Here, the skewed values we saw earlier are a bit clearer. We can also look at some other metrics of the fit; **mean squared error (MSE)** and **mean absolute deviation (MAD)** are two common metrics. Let's define each one in Python and use them.

```
def MSE(target, predictions):
    squared_deviation = np.power(target - predictions, 2)
    return np.mean(squared_deviation)

MSE(boston.target, predictions)

21.897779217687503

def MAD(target, predictions):
    absolute_deviation = np.abs(target - predictions)
    return np.mean(absolute_deviation)

MAD(boston.target, predictions)

3.2729446379969205
```

5. Now that you have seen the formulas in NumPy to get the errors, you can also use the `sklearn.metrics` module to get the errors quickly:

```
from sklearn.metrics import mean_absolute_error, mean_squared_error

print 'MAE: ', mean_absolute_error(boston.target, predictions)
print 'MSE: ', mean_squared_error(boston.target, predictions)

'MAE: ', 3.2729446379969205
'MSE: ', 21.897779217687503
```

How it works...

The formula for MSE is very simple:

$$E((y_{truth} - y_{predicted})^2)$$

It takes each predicted value's deviance from the actual value, squares it, and then averages all the squared terms. This is actually what we optimized to find the best set of coefficients for linear regression. The Gauss-Markov theorem actually guarantees that the solution to linear regression is the best in the sense that the coefficients have the smallest expected squared error and are unbiased. In the next recipe, we'll look at what happens when we're OK with our coefficients being biased. MAD is the expected error for the absolute errors:

$$E(|y_{truth} - y_{predicted}|)$$

MAD isn't used when fitting linear regression, but it's worth taking a look at. Why? Think about what each one is doing and which errors are more important in each case. For example, with MSE, the larger errors get penalized more than the other terms because of the square term. Outliers have the potential to skew results substantially.

There's more...

One thing that's been glossed over a bit is the fact that coefficients themselves are random variables, therefore, they have a distribution. Let's use bootstrapping to look at the distribution of the coefficient for the crime rate. Bootstrapping is a very common technique to get an understanding of the uncertainty of an estimate:

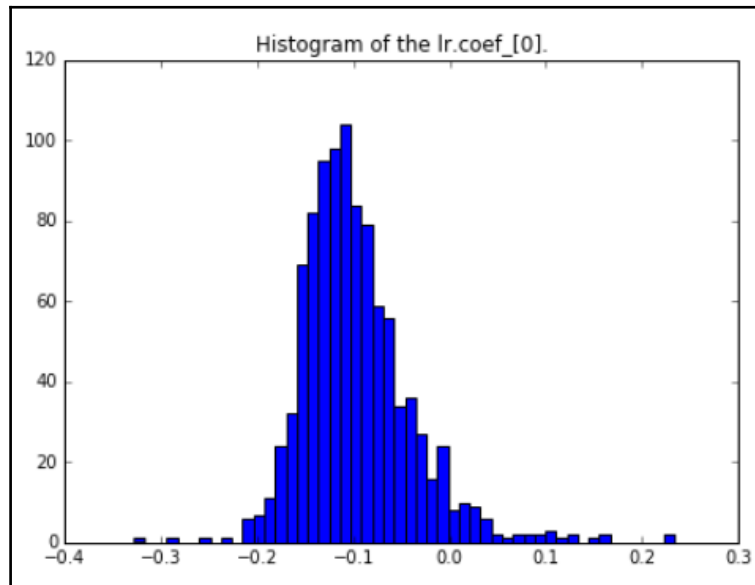
```
n_bootstraps = 1000
len_boston = len(boston.target)
subsample_size = np.int(0.5*len_boston)

subsample = lambda: np.random.choice(np.arange(0,
len_boston), size=subsample_size)
coefs = np.ones(n_bootstraps) #pre-allocate the space for the coefs
for i in range(n_bootstraps):
    subsample_idx = subsample()
    subsample_X = boston.data[subsample_idx]
    subsample_y = boston.target[subsample_idx]
    lr.fit(subsample_X, subsample_y)
    coefs[i] = lr.coef_[0]
```

Now, we can look at the distribution of the coefficient:

```
import matplotlib.pyplot as plt
f = plt.figure(figsize=(7, 5))
ax = f.add_subplot(111)
ax.hist(coefs, bins=50)
ax.set_title("Histogram of the lr.coef_[0].")
```

The following is the histogram that gets generated:



We might also want to look at the bootstrapped confidence interval:

```
np.percentile(coefs, [2.5, 97.5])

array([-0.18497204,  0.03231267])
```

This is interesting; there's actually reason to believe that the crime rate might not have an impact on home prices. Notice how zero is within the **confidence interval (CI)** between -0.18 and 0.03, which means that it may not play a role. It's also worth pointing out that bootstrapping can potentially lead to better estimations for coefficients, because the bootstrapped mean with convergence to the true mean is faster than finding the coefficient using regular estimation.

Using ridge regression to overcome linear regression's shortfalls

In this recipe, we'll learn about ridge regression. It is different from vanilla linear regression; it introduces a regularization parameter to shrink coefficients. This is useful when the dataset has collinear factors.



Ridge regression is actually so powerful in the presence of collinearity that you can model polynomial features: vectors x , x^2 , x^3 , ... which are highly collinear and correlated.

Getting ready

Let's load a dataset that has a low effective rank and compare ridge regression with linear regression by way of the coefficients. If you're not familiar with rank, it's the smaller of the linearly independent columns and the linearly independent rows. One of the assumptions of linear regression is that the data matrix is full rank.

How to do it...

1. First, use `make_regression` to create a simple dataset with three predictors, but an `effective_rank` of 2. Effective rank means that, although technically the matrix is full rank, many of the columns have a high degree of collinearity:

```
from sklearn.datasets import make_regression
reg_data, reg_target = make_regression(n_samples=2000, n_features=3,
effective_rank=2, noise=10)
```

2. First, let's take a look at regular linear regression with bootstrapping from the previous chapter:

```
import numpy as np
n_bootstraps = 1000
len_data = len(reg_data)
subsample_size = np.int(0.5*len_data)
subsample = lambda: np.random.choice(np.arange(0,
len_data), size=subsample_size)

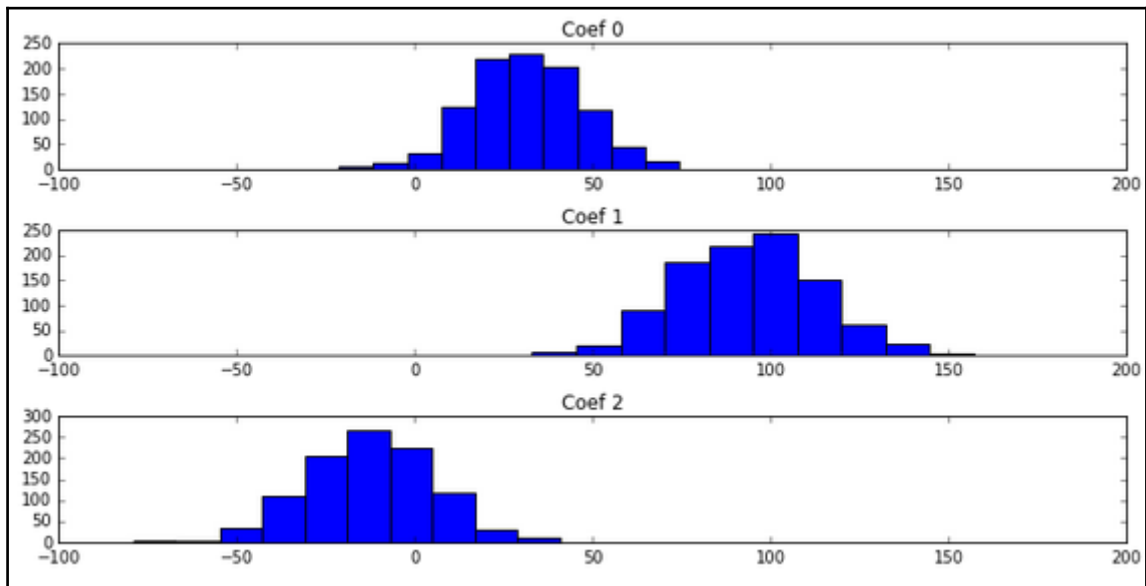
coefs = np.ones((n_bootstraps, 3))
```

```

for i in range(n_bootstraps):
    subsample_idx = subsample()
    subsample_X = reg_data[subsample_idx]
    subsample_y = reg_target[subsample_idx]
    lr.fit(subsample_X, subsample_y)
    coefs[i][0] = lr.coef_[0]
    coefs[i][1] = lr.coef_[1]
    coefs[i][2] = lr.coef_[2]

```

3. Visualize the coefficients:



4. Perform the same procedure with ridge regression:

```

from sklearn.linear_model import Ridge
r = Ridge()
n_bootstraps = 1000
len_data = len(reg_data)
subsample_size = np.int(0.5*len_data)
subsample = lambda: np.random.choice(np.arange(0,
len_data), size=subsample_size)

coefs_r = np.ones((n_bootstraps, 3))
for i in range(n_bootstraps):
    subsample_idx = subsample()
    subsample_X = reg_data[subsample_idx]
    subsample_y = reg_target[subsample_idx]

```



```
r.fit(subsample_X, subsample_y)
coefs_r[i][0] = r.coef_[0]
coefs_r[i][1] = r.coef_[1]
coefs_r[i][2] = r.coef_[2]
```

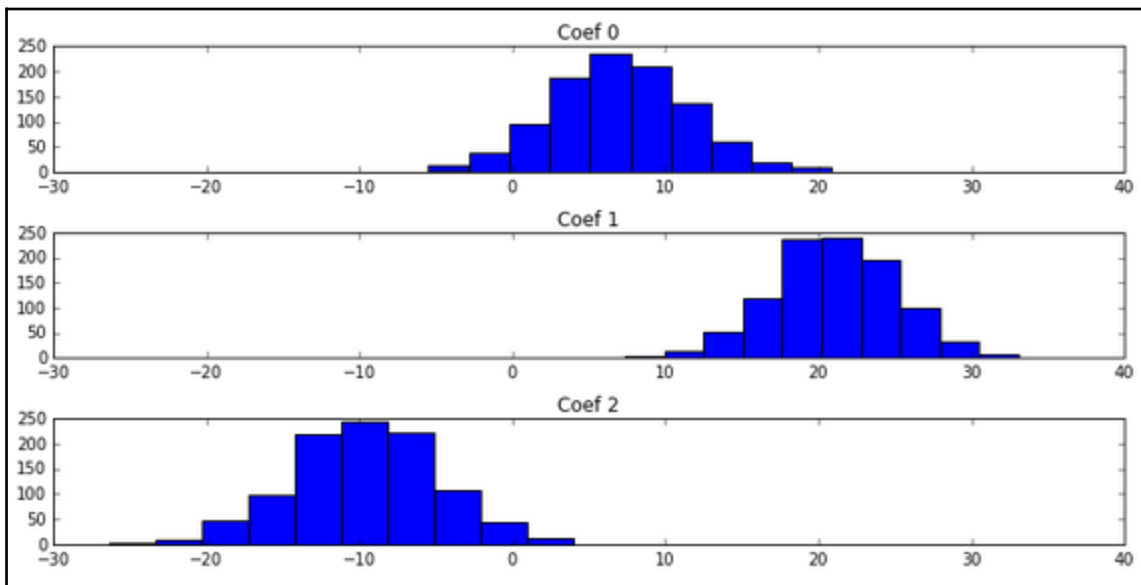
5. Visualize the results:

```
import matplotlib.pyplot as plt
plt.figure(figsize=(10, 5))

ax1 = plt.subplot(311, title='Coef 0')
ax1.hist(coefs_r[:,0])

ax2 = plt.subplot(312, sharex=ax1, title='Coef 1')
ax2.hist(coefs_r[:,1])

ax3 = plt.subplot(313, sharex=ax1, title='Coef 2')
ax3.hist(coefs_r[:,2])
plt.tight_layout()
```



Don't let the similar width of the plots fool you; the coefficients for ridge regression are much closer to zero.

6. Let's look at the average spread between the coefficients:

```
np.var(coefs, axis=0)

array([ 228.91620444,  380.43369673,  297.21196544])
```

So, on average, the coefficients for linear regression are much higher than the ridge regression coefficients. This difference is the bias in the coefficients (forgetting, for a second, the potential bias of the linear regression coefficients). So then, what is the advantage of ridge regression?

7. Well, let's look at the variance of our coefficients:

```
np.var(coefs_r, axis=0)

array([ 19.28079241,  15.53491973,  21.54126386])
```

The variance has been dramatically reduced. This is the bias-variance trade-off that is so often discussed in machine learning. The next recipe will introduce how to tune the regularization parameter in ridge regression, which is at the heart of this trade-off.

Optimizing the ridge regression parameter

Once you start using ridge regression to make predictions or learn about relationships in the system you're modeling, you'll start thinking about the choice of alpha.

For example, using ordinary least squares (OLS) regression might show a relationship between two variables; however, when regularized by an alpha, the relationship is no longer significant. This can be a matter of whether a decision needs to be taken.

Getting ready

Through cross-validation, we will tune the alpha parameter of ridge regression. If you remember, in ridge regression, the gamma parameter is typically represented as alpha in scikit-learn when calling `RidgeRegression`; so, the question that arises is what is the best alpha? Create a regression dataset, and then let's get started:

```
from sklearn.datasets import make_regression
reg_data, reg_target = make_regression(n_samples=100, n_features=2,
effective_rank=1, noise=10)
```

How to do it...

In the `linear_models` module, there is an object called `RidgeCV`, which stands for ridge cross-validation. This performs a cross-validation similar to **leave-one-out cross-validation (LOOCV)**.

1. Under the hood, it's going to train the model for all samples except one. It'll then evaluate the error in predicting this one test case:

```
from sklearn.linear_model import RidgeCV
rcv = RidgeCV(alphas=np.array([.1, .2, .3, .4]))
rcv.fit(reg_data, reg_target)
```

2. After we fit the regression, the `alpha` attribute will be the best alpha choice:

```
rcv.alpha_

0.10000000000000001
```

3. In the previous example, it was the first choice. We might want to hone in on something around `.1`:

```
rcv2 = RidgeCV(alphas=np.array([.08, .09, .1, .11, .12]))
rcv2.fit(reg_data, reg_target)

rcv2.alpha_

0.080000000000000002
```

We could continue this hunt, but hopefully, the mechanics are clear.

How it works...

The mechanics might be clear, but we should talk a little more about why and define what was meant by best. At each step in the cross-validation process, the model scores an error against the test sample. By default, it's essentially a squared error.

We can force the `RidgeCV` object to store the cross-validation values; this will let us visualize what it's doing:

```
alphas_to_test = np.linspace(0.01, 1)
rcv3 = RidgeCV(alphas=alphas_to_test, store_cv_values=True)
rcv3.fit(reg_data, reg_target)
```

As you can see, we test a bunch of points (50 in total) between 0.01 and 1. Since we passed `store_cv_values` as `True`, we can access these values:

```
rcv3.cv_values_.shape  
  
(100L, 50L)
```

So, we had 100 values in the initial regression and tested 50 different alpha values. We now have access to the errors of all 50 values. So, we can now find the smallest mean error and choose it as alpha:

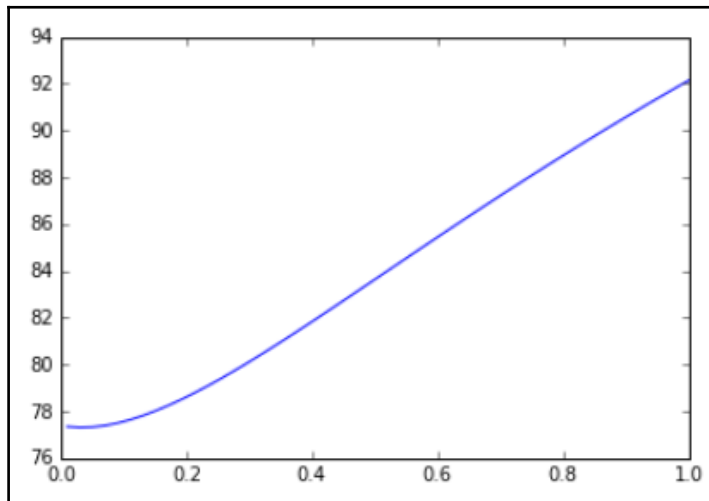
```
smallest_idx = rcv3.cv_values_.mean(axis=0).argmin()  
alphas_to_test[smallest_idx]  
  
0.030204081632653063
```

This matches the best value found by the `rcv3` instance of the class `RidgeCV`:

```
rcv3.alpha_  
  
0.030204081632653063
```

It's also worthwhile visualizing what's going on. In order to do that, we'll plot the mean for all 50 test alphas:

```
plt.plot(alphas_to_test, rcv3.cv_values_.mean(axis=0))
```



There's more...

If we want to use our own scoring function, we can do that as well. Since we looked up MAD before, let's use it to score the differences. First, we need to define our loss function. We will import it from `sklearn.metrics`:

```
from sklearn.metrics import mean_absolute_error
```

After we define the loss function, we can employ the `make_scorer` function in `sklearn`. This will take care of standardizing our function so that scikit's objects know how to use it. Also, because this is a loss function and not a score function, the lower the better, and thus the need to let `sklearn` flip the sign to turn this from a maximization problem into a minimization problem:

```
from sklearn.metrics import make_scorer
MAD_scorer = make_scorer(mean_absolute_error, greater_is_better=False)
```

Continue as before to find the minimum negative MAD score:

```
rcv4 = RidgeCV(alphas=alphas_to_test, store_cv_values=True,
               scoring=MAD_scorer)
rcv4.fit(reg_data, reg_target)
smallest_idx = rcv4.cv_values_.mean(axis=0).argmin()
```

Look at the lowest score:

```
rcv4.cv_values_.mean(axis=0)[smallest_idx]

-0.021805192650070034
```

It occurs at the alpha of 0.01:

```
alphas_to_test[smallest_idx]

0.01
```

Bayesian ridge regression

Additionally, scikit-learn contains Bayesian ridge regression, which allows for easy estimates of confidence intervals. (Note that obtaining the following Bayesian ridge confidence intervals specifically requires scikit-learn Version 0.19.0 or higher.)

Create a line with a slope of 3 and no intercept for simplicity:

```
X = np.linspace(0, 5)
y_truth = 3 * X
y_noise = np.random.normal(0, 0.5, len(y_truth)) #normally distributed
noise with mean 0 and spread 0.1
y_noisy = (y_truth + y_noise)
```

Import, instantiate, and fit the Bayesian ridge model. Note that the one-dimensional x and y variables have to be reshaped:

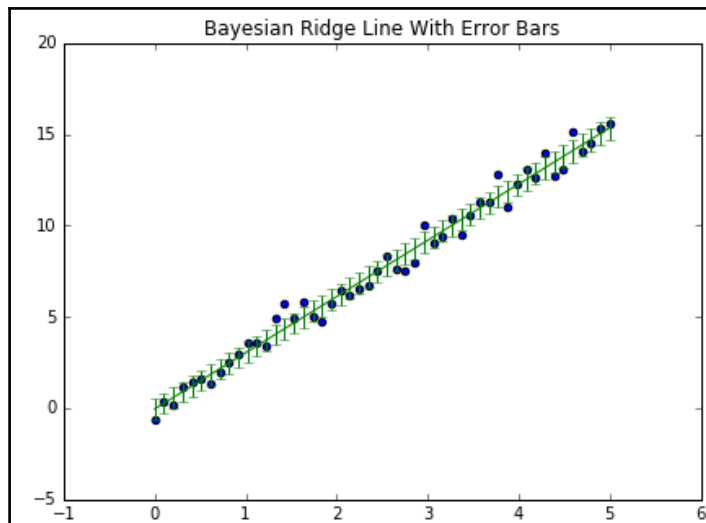
```
from sklearn.linear_model import BayesianRidge
br_inst = BayesianRidge().fit(X.reshape(-1, 1), y_noisy)
```

Write the following to get the error estimates on the regularized linear regression:

```
y_pred, y_err = br_inst.predict(X.reshape(-1, 1), return_std=True)
```

Plot the results. The noisy data is the blue dots and the green lines approximate it:

```
plt.figure(figsize=(7, 5))
plt.scatter(X, y_noisy)
plt.title("Bayesian Ridge Line With Error Bars")
plt.errorbar(X, y_pred, y_err, color='green')
```



As a final aside on Bayesian ridge, you can perform hyperparameter optimization on the parameters `alpha_1`, `alpha_2`, `lambda_1`, and `lambda_2` using a cross-validated grid search.

Using sparsity to regularize models

The **least absolute shrinkage and selection operator (LASSO)** method is very similar to ridge regression and **least angle regression (LARS)**. It's similar to ridge regression in the sense that we penalize our regression by an amount, and it's similar to LARS in that it can be used as a parameter selection, typically leading to a sparse vector of coefficients. Both LASSO and LARS get rid of a lot of the features of the dataset, which is something you might or might not want to do depending on the dataset and how you apply it. (Ridge regression, on the other hand, preserves all features, which allows you to model polynomial functions or complex functions with correlated features.)

Getting ready

To be clear, LASSO regression is not a panacea. There can be computation consequences to using LASSO regression. As we'll see in this recipe, we'll use a loss function that isn't differential, and therefore requires special, and more importantly, performance-impairing workarounds.

How to do it...

The steps involved in performing LASSO regression are as follows:

1. Let's go back to the trusty `make_regression` function and create a dataset with the same parameters:

```
import numpy as np
from sklearn.datasets import make_regression
reg_data, reg_target = make_regression(n_samples=200,
n_features=500, n_informative=5, noise=5)
```

2. Next, we need to import the `Lasso` object:

```
from sklearn.linear_model import Lasso
lasso = Lasso()
```

3. LASSO contains many parameters, but the most interesting parameter is `alpha`. It scales the penalization term of the `Lasso` method. For now, leave it as one. As an aside, and much like ridge regression, if this term is zero, LASSO is equivalent to linear regression:

```
lasso.fit(reg_data, reg_target)
```

4. Again, let's see how many of the coefficients remain nonzero:

```
np.sum(lasso.coef_ != 0)
```

```
7
```

```
lasso_0 = Lasso(0)
lasso_0.fit(reg_data, reg_target)
np.sum(lasso_0.coef_ != 0)
```

```
500
```

None of our coefficients turn out to be zero, which is what we expected. Actually, if you run this, you might get a warning from scikit-learn that advises you to choose `LinearRegression`.

How it works...

LASSO cross-validation – LASSOCV

Choosing the most appropriate `lambda` is a critical problem. We can specify the `lambda` ourselves or use cross-validation to find the best choice given the data at hand:

```
from sklearn.linear_model import LassoCV
lassocv = LassoCV()
lassocv.fit(reg_data, reg_target)
```


The LASSOCV will have, as an attribute, the most appropriate lambda. scikit-learn mostly uses alpha in its notation, but the literature uses lambda:

```
lassocv.alpha_  
  
0.75182924196508782
```

The number of coefficients can be accessed in the regular manner:

```
lassocv.coef_[ :5]  
  
array([-0., -0.,  0.,  0., -0.] )
```

Letting LASSOCV choose the appropriate best fit leaves us with 15 nonzero coefficients:

```
np.sum(lassocv.coef_ != 0)  
  
15
```

LASSO for feature selection

LASSO can often be used for feature selection for other methods. For example, you might run LASSO regression to get the appropriate number of features, and then use those features in another algorithm.

To get the features we want, create a masking array based on the columns that aren't zero, and then filter out the nonzero columns to keep the features we want:

```
mask = lasso.coef_ != 0  
new_reg_data = reg_data[:, mask]  
new_reg_data.shape  
  
(200L, 15L)
```

Taking a more fundamental approach to regularization with LARS

To borrow from Gilbert Strang's evaluation of the Gaussian elimination, LARS is an idea you probably would've considered eventually had it not already been discovered by Efron, Hastie, Johnstone, and Tibshirani in their work [1].

Getting ready

LARS is a regression technique that is well suited to high-dimensional problems, that is, $p \gg n$, where p denotes the columns or features and n is the number of samples.

How to do it...

1. First, import the necessary objects. The data we use will have 200 data points and 500 features. We'll also choose low noise and a small number of informative features:

```
from sklearn.datasets import make_regression
reg_data, reg_target = make_regression(n_samples=200,
n_features=500, n_informative=10, noise=2)
```

2. Since we used 10 informative features, let's also specify that we want 10 nonzero coefficients in LARS. We will probably not know the exact number of informative features beforehand, but it's useful for learning purposes:

```
from sklearn.linear_model import Lars
lars = Lars(n_nonzero_coefs=10)
lars.fit(reg_data, reg_target)
```

3. We can then verify that LARS returns the correct number of nonzero coefficients:

```
np.sum(lars.coef_ != 0)

10
```

4. The question then is why it is more useful to use a smaller number of features. To illustrate this, let's hold out half of the data and train two LARS models, one with 12 nonzero coefficients and another with no predetermined amount. We use 12 here because we might have an idea of the number of important features, but we might not be sure of the exact number:

```
train_n = 100
lars_12 = Lars(n_nonzero_coefs=12)
lars_12.fit(reg_data[:train_n], reg_target[:train_n])
lars_500 = Lars() # it's 500 by default
lars_500.fit(reg_data[:train_n], reg_target[:train_n]);

np.mean(np.power(reg_target[train_n:] -
lars_12.predict(reg_data[train_n:]), 2))
```

5. Now, to see how well each feature fits the unknown data, do the following:

```
87.115080975821513

np.mean(np.power(reg_target[train_n:] -
lars_500.predict(reg_data[train_n:]), 2))

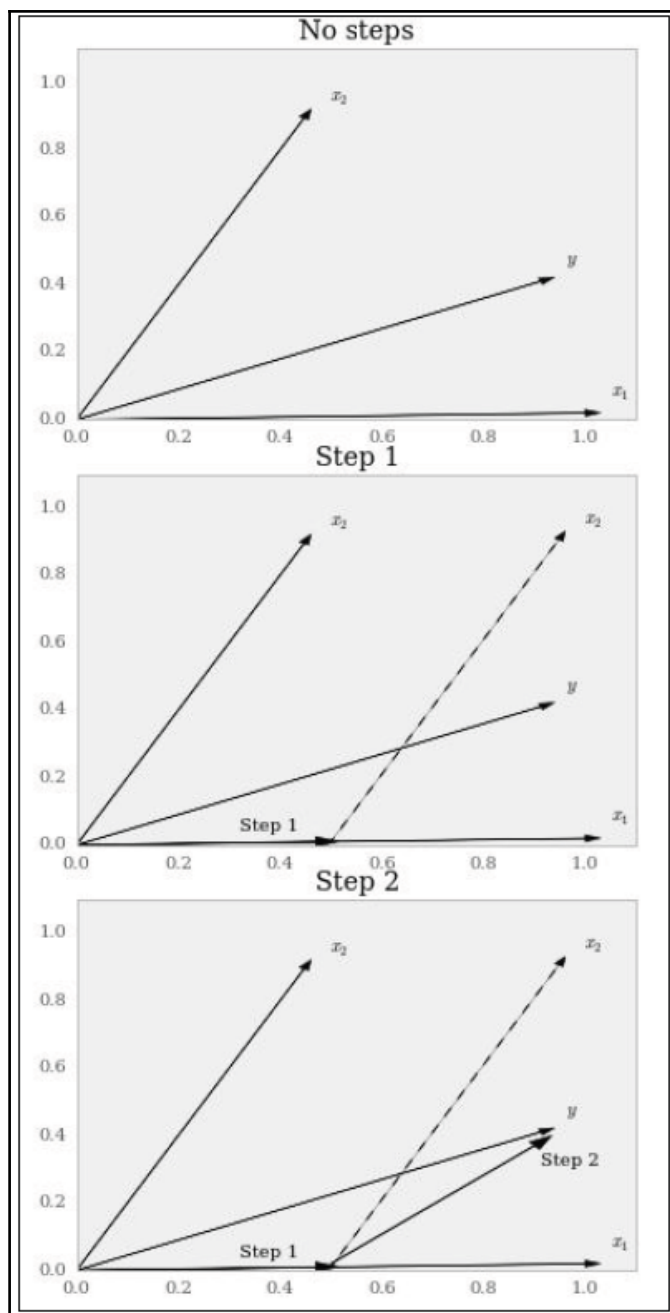
2.1212501492030518e+41
```

Look again if you missed it; the error on the test set was clearly very high. Herein lies the problem with high-dimensional datasets; given a large number of features, it's typically not too difficult to get a model of good fit on the train sample, but overfitting becomes a huge problem.

How it works...

LARS works by iteratively choosing features that are correlated with the residuals. Geometrically, correlation is effectively the least angle between the feature and the residuals; this is how LARS got its name.

After choosing the first feature, LARS will continue to move in the least angle direction until a different feature has the same amount of correlation with the residuals. Then, LARS will begin to move in the combined direction of both features. To visualize this, consider the following graph:



So, we move along x_1 until we get to the point where the pull on x_1 by y is the same as the pull on x_2 by y . When this occurs, we move along the path that is equal to the angle between x_1 and x_2 divided by two.

There's more...

Much in the same way as we used cross-validation to tune ridge regression, we can do the same with LARS:

```
from sklearn.linear_model import LarsCV
lcv = LarsCV()
lcv.fit(reg_data, reg_target)
```

Using cross-validation will help us to determine the best number of nonzero coefficients to use. Here, it turns out to be as shown:

```
np.sum(lcv.coef_ != 0)
```

```
23
```

References

1. Bradley Efron, Trevor Hastie, Iain Johnstone, and Robert Tibshirani, *Least angle regression*, The Annals of Statistics 32(2) 2004: pp. 407–499, doi:10.1214/0090536040000000067, MR2060166.

5

Linear Models – Logistic Regression

In this chapter, we will cover the following recipes:

- Loading data from the UCI repository
- Viewing the Pima Indians diabetes dataset with pandas
- Looking at the UCI Pima Indians dataset web page
- Machine learning with logistic regression
- Examining logistic regression errors with a confusion matrix
- Varying the classification threshold in logistic regression
- Receiver operating characteristic – ROC analysis
- Plotting an ROC curve without context
- Putting it all together – UCI breast cancer dataset

Introduction

Linear regression is a very old method and part of traditional statistics. *Machine learning linear regression* involves a training and testing set. This way, it can be compared by utilizing *cross-validation* with other models and algorithms. *Traditional linear regression* trains and tests on the whole dataset. This is still a common practice, possibly because linear regression tends to underfit rather than overfit.

Using linear methods for classification – logistic regression

As seen in Chapter 1, *High-Performance Machine Learning – NumPy*, logistic regression is a classification method. In some contexts, it is a regressor as it computes the real number probability of a class before assigning a categorical classification prediction. With this in mind, let's explore the Pima Indians diabetes dataset provided by the **University of California, Irvine (UCI)**.

Loading data from the UCI repository

The first dataset we will load is the Pima Indians diabetes dataset. This will require access to the internet. The dataset is available thanks to Sigillito V. (1990), UCI machine learning repository (<https://archive.ics.uci.edu/ml/machine-learning-databases/pima-indians-diabetes/pima-indians-diabetes.data>), Laurel, MD at Johns Hopkins University, applied physics laboratory.



The first thing in your mind if you are an open source veteran is, what is the license/permission to this database? This is a very important issue. The UCI repository has a use policy that requires citation of the database whenever we are using it. We are allowed to use it but we must give them proper credit for their great help and provide a citation.

How to do it...

1. Go to IPython and import pandas:

```
import pandas as pd
```

2. Type the web location of the Pima Indians diabetes dataset as a string as follows:

```
data_web_address =  
"https://archive.ics.uci.edu/ml/machine-learning-databases/pima-indians-diabetes/pima-indians-diabetes.data"
```

3. Type the column names of the data in a list:

```
column_names = ['pregnancy_x',
                'plasma_con',
                'blood_pressure',
                'skin_mm',
                'insulin',
                'bmi',
                'pedigree_func',
                'age',
                'target']
```

4. Store the feature names as a list. Exclude the `target` column, the last column name in `column_names`, because it is not a feature:

```
feature_names = column_names[:-1]
```

5. Make a pandas dataframe to store the input data:

```
all_data = pd.read_csv(data_web_address , names=column_names)
```

Viewing the Pima Indians diabetes dataset with pandas

How to do it...

1. You can view the data in various ways. View the top of the dataframe:

```
all_data.head()
```

	pregnancy_x	plasma_con	blood_pressure	skin_mm	insulin	bmi	pedigree_func	age	target
0	6	148	72	35	0	33.6	0.627	50	1
1	1	85	66	29	0	26.6	0.351	31	0
2	8	183	64	0	0	23.3	0.672	32	1
3	1	89	66	23	94	28.1	0.167	21	0
4	0	137	40	35	168	43.1	2.288	33	1

2. Nothing seems amiss here, except possibly an insulin level of zero. Is this possible? What about the `skin_mm` variable? Can that be zero? Make a note about it as a comment in your IPython:

```
#Is an insulin level of 0 possible? Is a skin_mm of 0 possible?
```

3. Get a rough overview of the dataframe with the `describe()` method:

```
all_data.describe()
```

	pregnancy_x	plasma_con	blood_pressure	skin_mm	insulin	bmi	pedigree_func	age	target
count	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000	768.000000
mean	3.845052	120.894531	69.105469	20.536458	79.799479	31.992578	0.471876	33.240885	0.348958
std	3.369578	31.972618	19.355807	15.952218	115.244002	7.884160	0.331329	11.760232	0.476951
min	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.078000	21.000000	0.000000
25%	1.000000	99.000000	62.000000	0.000000	0.000000	27.300000	0.243750	24.000000	0.000000
50%	3.000000	117.000000	72.000000	23.000000	30.500000	32.000000	0.372500	29.000000	0.000000
75%	6.000000	140.250000	80.000000	32.000000	127.250000	36.600000	0.626250	41.000000	1.000000
max	17.000000	199.000000	122.000000	99.000000	846.000000	67.100000	2.420000	81.000000	1.000000

4. Make a note again in your notebook about additional zeros:

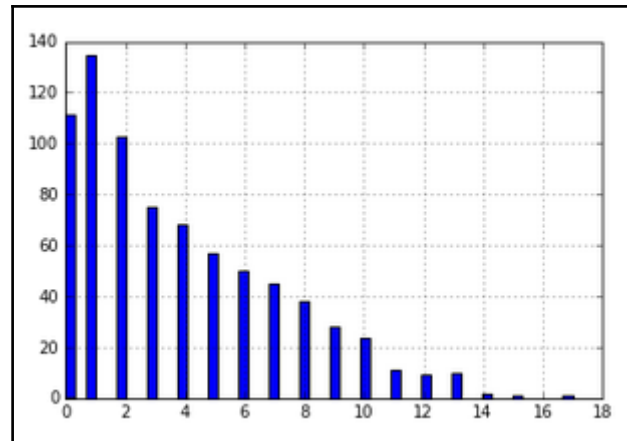
```
#The features plasma_con, blood_pressure, skin_mm, insulin, bmi
have 0s as values. These values could be physically impossible.
```

5. Draw a histogram of the `pregnancy_x` variable. Set the `hist()` method variable bins equal to 50 for more bins and a higher resolution in the image; otherwise, the image is hard to read:

```
#If within a notebook, include this line to visualize within the
notebook.
```

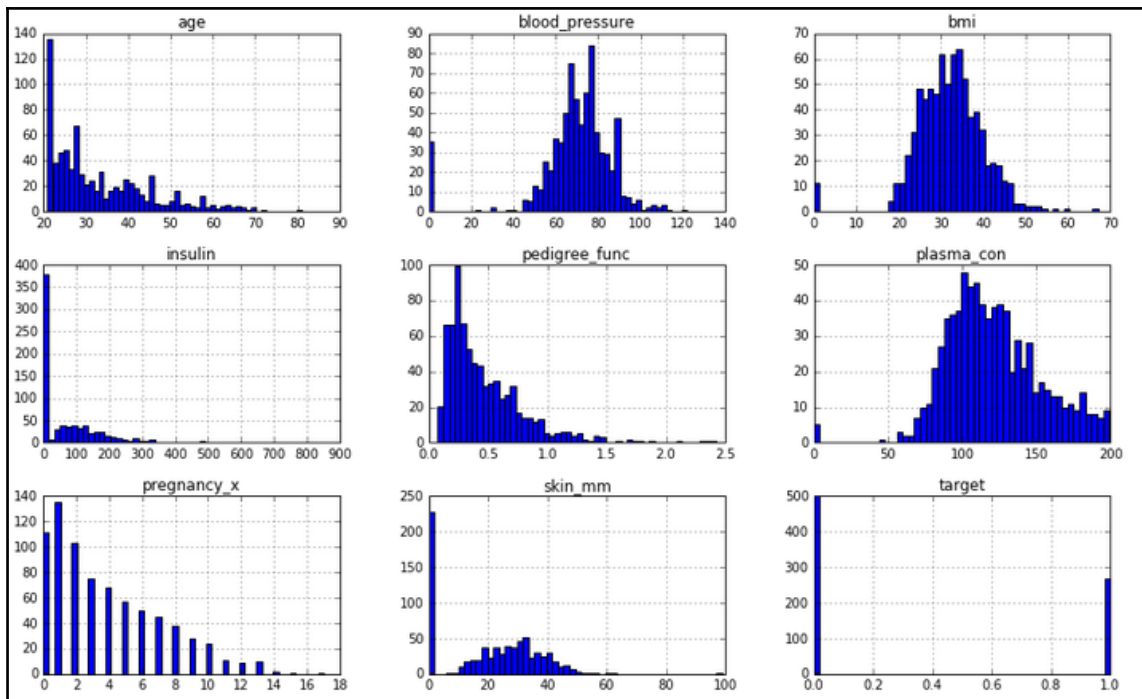
```
%matplotlib inline
```

```
#The default is bins=10 which is hard to read in the visualization.
all_data.pregnancy_x.hist(bins=50)
```



6. Make histograms for all columns of the dataframe. Change `figsize` within the method to the tuple `(15, 9)` and `bins` to 50 again; otherwise, it is hard to read the image:

```
all_data.hist(figsize=(15, 9), bins=50)
```





`blood_pressure` and `bmi` look like normal distributions aside from the anomalous zeros.

The `pedigree_func` and `plasma_con` variables are skewed-normal (possibly log-normal). The `age` and `pregnancy_x` variables are decaying in some way. The `insulin` and `skin_mm` variables look like they could be normally distributed except for the many values of zero.

7. Finally, note the class imbalance in the `target` variable. Reexamine that imbalance with the `value_counts()` pandas series method:

```
all_data.target.value_counts()

0      500
1      268
Name: target, dtype: int64
```

There are more cases where the person is described by category zero instead of category one.

Looking at the UCI Pima Indians dataset web page

We did some exploratory analysis to get a rough understanding of the data. Now we will read the UCI Pima Indians dataset documentation.

How to do it...

View the citation policy

1. Go to <https://archive.ics.uci.edu/ml/datasets/pima+indians+diabetes>.
2. Here is all the information about the UCI Pima Indians diabetes dataset. First, scroll down to the bottom of the page and look at their citation policy. The diabetes dataset has the general UCI citation policy available at; https://archive.ics.uci.edu/ml/citation_policy.html.

3. The general policy says that to publish material using the dataset, please cite the UCI repository.

Read about missing values and context

4. The top of the page has important links and an abstract of the dataset. The abstract mentions there are missing values in the dataset:

Pima Indians Diabetes Data Set

Download: [Data Folder](#), [Data Set Description](#)

Abstract: From National Institute of Diabetes and Digestive and Kidney Diseases; Includes cost data (donated by Peter Turney)

Data Set Characteristics:	Multivariate	Number of Instances:	768	Area:	Life
Attribute Characteristics:	Integer, Real	Number of Attributes:	8	Date Donated	1990-05-09
Associated Tasks:	Classification	Missing Values?	Yes	Number of Web Hits:	282152

5. Below the abstract, there is a description of the attributes (this is how I came up with the names for the columns at the beginning):

Attribute Information:

1. Number of times pregnant
2. Plasma glucose concentration a 2 hours in an oral glucose tolerance test
3. Diastolic blood pressure (mm Hg)
4. Triceps skin fold thickness (mm)
5. 2-Hour serum insulin (mu U/ml)
6. Body mass index (weight in kg/(height in m)²)
7. Diabetes pedigree function
8. Age (years)
9. Class variable (0 or 1)

6. What do the class variables mean anyway? What does the zero or one mean in the target? To figure this out, click on the **Data Set Description** link above the abstract. Scroll to point nine on the page, which yields the desired information:

```
9. Class Distribution: (class value 1 is interpreted as "tested positive for
diabetes")

Class Value  Number of instances
0           500
1           268
```

This means that a **1** refers to a positive for diabetes. This is important information and with regard to this data analysis, provides a context.

7. Finally, there is a disclaimer noting that: **As pointed out by a repository user, this cannot be true: there are zeros in places where they are biologically impossible, such as the blood pressure attribute. It seems very likely that zero values encode missing data.**

Thus, we were right in suspecting some of the impossible zeros in the data exploration phase. Many datasets have corrupt or missing values.

Machine learning with logistic regression

You are familiar with the steps of training and testing a classifier. With logistic regression, we will do the following:

- Load data into feature and target arrays, x and y , respectively
- Split the data into training and testing sets
- Train the logistic regression classifier on the training set
- Test the performance of the classifier on the test set

Getting ready

Define X, y – the feature and target arrays

Let's start predicting with scikit-learn's logistic regression. Perform the necessary imports and set the input variables X and the target variable y:

```
import numpy as np
import pandas as pd

X = all_data[feature_names]
y = all_data['target']
```

How to do it...

Provide training and testing sets

1. Import `train_test_split` to create testing and training sets for both X and y: the inputs and target. Note the `stratify=y`, which stratifies the categorical variable y. This means that there are the same proportions of zeros and ones in both `y_train` and `y_test`:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.2, random_state=7, stratify=y)
```

Train the logistic regression

2. Now import the `LogisticRegression` and fit it to the training data:

```
from sklearn.linear_model import LogisticRegression
lr = LogisticRegression()
lr.fit(X_train, y_train)
```

3. Make a prediction on the test set and store it as `y_pred`:

```
y_pred = lr.predict(X_test)
```

Score the logistic regression

4. Check the accuracy of the prediction with `accuracy_score`, the percentage of classifications that are correct:

```
from sklearn.metrics import accuracy_score
accuracy_score(y_test, y_pred)

0.74675324675324672
```

So, we have obtained a score, but is this score the best measure we can use under these circumstances? Can we do better? Perhaps yes. Look at a confusion matrix of the results as follows.

Examining logistic regression errors with a confusion matrix

Getting ready

Import and view the confusion matrix for the logistic regression we constructed:

```
from sklearn.metrics import confusion_matrix
confusion_matrix(y_test, y_pred, labels = [1,0])

array([[27, 27],
       [12, 88]])
```

I passed three arguments to the confusion matrix:

- `y_test`: The test target set
- `y_pred`: Our logistic regression predictions
- `labels`: References to a positive class

The `labels = [1,0]` means that the positive class is 1 and the negative class is 0. In the medical context, we found while exploring the Pima Indians diabetes dataset that class 1 tested positive for diabetes.

Here is the confusion matrix, again in pandas dataframe form:

	Predict: 1	Predict: 0
Actual: 1	27	27
Actual: 0	12	88

How to do it...

Reading the confusion matrix

The small array of numbers has the following meaning:

		Predictions	
		Predicted to have diabetes.	Predicted to not have diabetes.
Truth	Does not have Diabetes.	27 people were classified as having diabetes (1) correctly.	27 people were classified to not have diabetes although they do.
	Has Diabetes	12 people were classified to having diabetes without having it.	88 people were classified as not having diabetes (0) correctly.

The confusion matrix tells us a bit more about what occurred during classification, not only the accuracy score. The diagonal elements from upper-left to lower-right are correct classifications. There were $27 + 88 = 115$ correct classifications. Off that diagonal, $27 + 12 = 39$ mistakes were made in classification. Note that $115 / (115 + 39)$ yields the classifier accuracy again, of about 0.75.

Let us focus on the errors again. In the confusion matrix, 27 people were labelled as not having diabetes although they do. In a real-life context, this is a worse error than those who were thought to have diabetes but did not. The first set might go home in real-life and forget while the second set might be retested.

General confusion matrix in context

A general confusion matrix where the positive class refers to identifying a condition (diabetes in this case) thereby having a medical diagnosis context:

		Predictions	
		POSITIVE CLASS	NEGATIVE CLASS
Truth	POSITIVE CLASS	TRUE POSITIVE (TP)	FALSE NEGATIVE (FN)
	NEGATIVE CLASS	FALSE POSITIVE (FP)	TRUE NEGATIVE (TN)

Varying the classification threshold in logistic regression

Getting ready

We will use the fact that underlying the logistic regression classification, there is regression to minimize the number of times people were sent home for not having diabetes although they do. Do so by calling the `predict_proba()` method of the estimator:

```
y_pred_proba = lr.predict_proba(X_test)
```

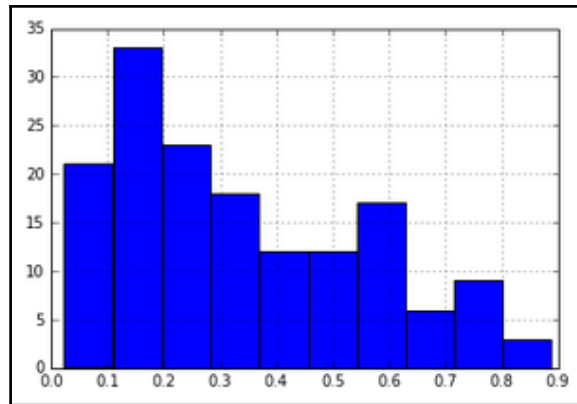
This yields an array of probabilities. View the array:

```
y_pred_proba
array([[ 0.87110309,  0.12889691],
       [ 0.83996356,  0.16003644],
       [ 0.81821721,  0.18178279],
       [ 0.73973464,  0.26026536],
       [ 0.80392034,  0.19607966], ...])
```

In the first row, a probability of about 0.87 is assigned to class 0 and a probability of 0.13 is assigned to 1. Note that, as probabilities, these numbers add up to 1. Because there are only two categories, this result can be viewed as a regressor, a real number that talks about the probability of the class being 1 (or 0). Visualize the probabilities of the class being 1 with a histogram.

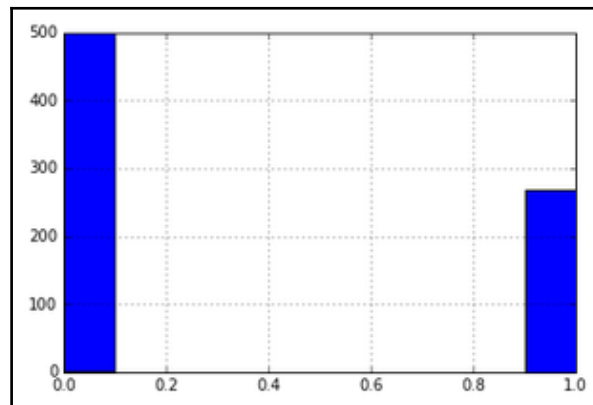
Take the second column of the array, turn it into a pandas series, and draw a histogram:

```
pd.Series(y_pred_proba[:,1]).hist()
```



In the probability histogram, high probabilities in regards to selecting 1 are fewer than low probabilities. For example, often the probability of selecting 1 is from 0.1 to 0.2. Within logistic regression, the algorithm will pick 1 by default only if the probability is greater than 0.5 or half. Now, contrast this with the target histogram at the beginning:

```
all_data['target'].hist()
```



In the following recipe, we will:

- Call the class method `y_pred_proba()`
- Use the `binarize` function with a specific threshold
- Look at the confusion matrix that is generated by the threshold

How to do it...

1. To select the classification class based on a threshold, use `binarize` from the `preprocessing` module. First import it:

```
from sklearn.preprocessing import binarize
```

2. Look at the first two columns of `y_pred_proba`:

```
array([[ 0.87110309,  0.12889691],
       [ 0.83996356,  0.16003644]
```

3. Then try `binarize` function on `y_pred_proba` with a threshold of 0.5. View the result:

```
y_pred_default = binarize(y_pred_proba, threshold=0.5)
y_pred_default

array([[ 1.,  0.],
       [ 1.,  0.],
       [ 1.,  0.],
       [ 1.,  0.],
       [ 1.,  0.],
       [ 1.,  0.]
```

4. The `binarize` function fills the array with 1 if values in `y_pred_proba` are greater than 0.5; otherwise it places a 0. In the first row, 0.87 is greater than 0.5 while 0.13 is not. So to binarize, replace the 0.87 with a 1 and the 0.13 with a 0. Now, take the first column of `y_pred_default`. View it:

```
y_pred_default[:,1]

array([ 0.,  0.,  0.,  0.,  0.,  0 ...
```

This recovers the decisions made by the default logistic regression classifier with threshold 0.5.

5. Trying the confusion matrix function on the NumPy array yields the first confusion matrix we encountered (note that the labels are chosen to be `[1, 0]` again):

```
confusion_matrix(y_test, y_pred_default[:,1], labels = [1,0])

array([[27, 27],
       [12, 88]])
```

6. Try a different threshold so that class 1 has a better chance of being selected. View its confusion matrix:

```
y_pred_low = binarize(y_pred_proba, threshold=0.2)
confusion_matrix(y_test, y_pred_low[:,1], labels=[1,0]) #positive
class is 1 again

array([[50,  4],
       [48, 52]])
```

By changing the threshold, we increased the likelihood of predicting class 1—increasing the size of the numbers in the first column of the confusion matrix. The first column now adds up to $50 + 48 = 98$. Before, the first column was $27 + 12 = 39$, a much lower number. Now only four people were classified to not have diabetes although they do. Note that this is a good thing in some contexts.

When the algorithm predicts zero, it is likely to be correct. When it predicts one, it tends to not work. Suppose you run a hospital. You might like this test because you rarely send someone home believing they do not have diabetes although they do. Whenever you send people home who do have diabetes, they cannot be treated earlier and incur greater costs to the hospital, insurance companies, and themselves.

You can measure the accuracy of the test when it predicts zero. Observe the second column of the confusion matrix, `[4, 52]`. In this situation, it is $52 / (52 + 4)$ or about 0.93 accurate. This is called the **negative predictive value (NPV)**. You can write a function to calculate NPV-based on the threshold:

```
from __future__ import division #In Python 2.x
import matplotlib.pyplot as plt

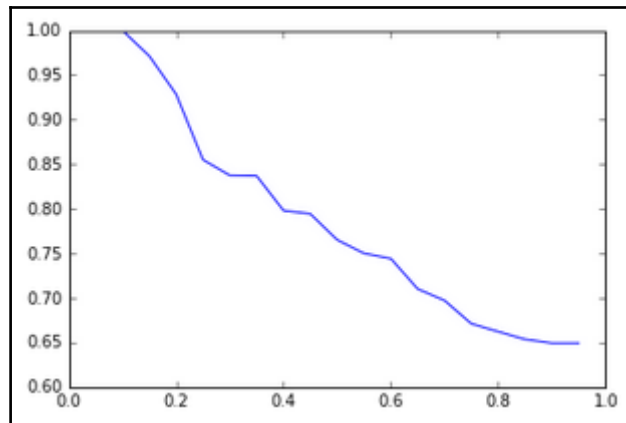
def npv_func(th):
    y_pred_low = binarize(y_pred_proba, threshold=th)

    second_column = confusion_matrix(y_test,
    y_pred_low[:,1], labels=[1,0])[:,1]
    npv = second_column[1]/second_column.sum()
```

```
    return npv  
  
npv_func(0.2)  
  
0.9285714285714286
```

Then plot it:

```
ths = np.arange(0,1,0.05)  
  
npvs = []  
for th in np.arange(0,1.00,0.05):  
    npvs.append(npv_func(th))  
plt.plot(ths,npvs)
```



Receiver operating characteristic – ROC analysis

Along the same lines of examining NPV, there are standard measures that examine cells within a confusion matrix.

Getting ready

Sensitivity

Sensitivity, like NPV in the previous section, is a mathematical function of the confusion matrix cells. Sensitivity is the proportion of people who took the test with a condition and were correctly labeled as having the condition, diabetes in this case:

$$\text{Sensitivity} = \frac{\text{People correctly labelled having diabetes}}{\text{All people who have diabetes}}$$

Mathematically, it is the ratio of patients correctly labeled as having a condition (TP) divided by the total number of people who actually have the condition (TP + FN). First, recall the confusion matrix cells. Focus on the **Truth** row, which corresponds to *all people who have diabetes*:

		Predictions	
		POSITIVE CLASS	NEGATIVE CLASS
Truth	POSITIVE CLASS	TRUE POSITIVE (TP)	FALSE NEGATIVE (FN)
	NEGATIVE CLASS	FALSE POSITIVE (FP)	TRUE NEGATIVE (TN)

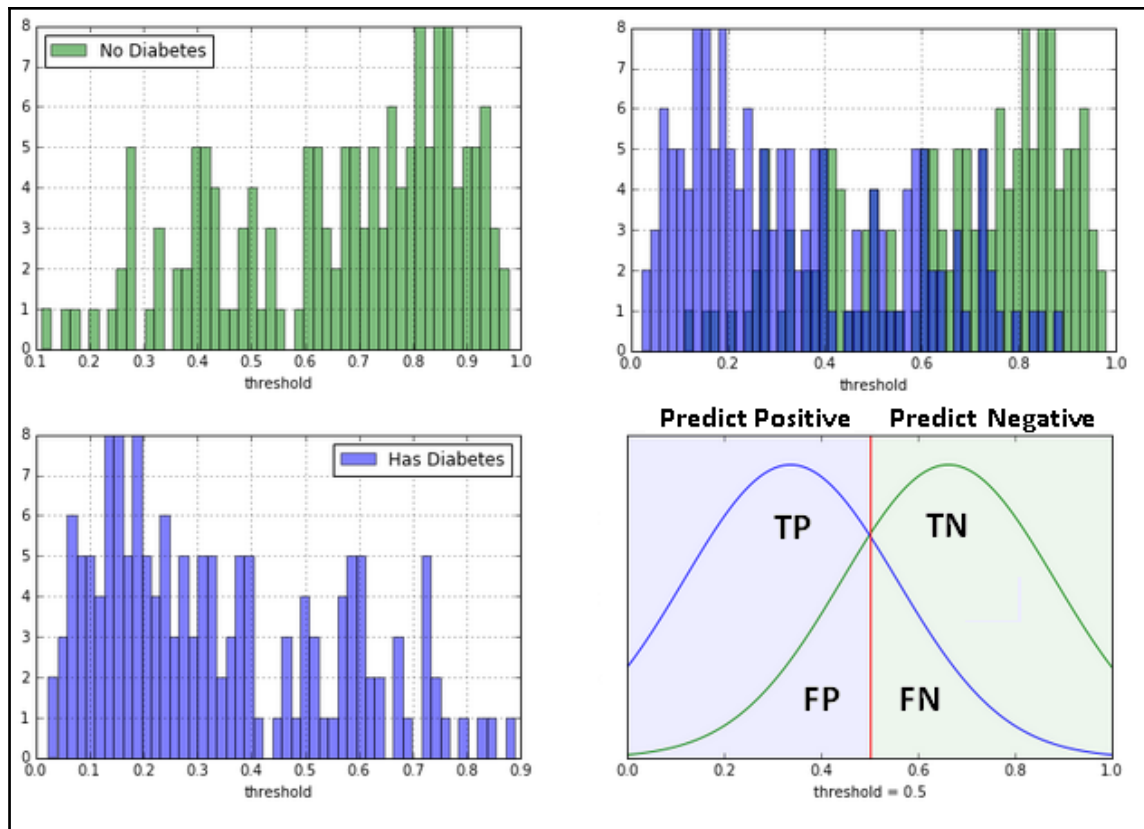
Consequently:

$$\text{Sensitivity} = \frac{\text{True Positive}}{\text{True Positive} + \text{False Negative}}$$

Another name for sensitivity is **true positive rate (TPR)**.

A visual perspective

Another perspective on the confusion matrix is very visual. Let us visualize both the positive class having diabetes and the negative class having no diabetes with histograms (on the left column in the next diagram). Each class roughly looks like a normal distribution. With SciPy, I can find the best fit normal distributions. Note on the bottom right that the threshold is set to 0.5, the default setting in the logistic regression. Observe how the threshold causes us to select, imperfectly, **false negatives (FN)** and **false positives (FP)**.



How to do it...

Calculating TPR in scikit-learn

1. scikit-learn has convenient functions for calculating the sensitivity or TPR for the logistic regression given a vector of probabilities of the positive class,

```
y_pred_proba[:,1]:
```

```
from sklearn.metrics import roc_curve
```

```
fpr, tpr, ths = roc_curve(y_test, y_pred_proba[:,1])
```

Here, given the positive class vector, the `roc_curve` function in scikit-learn yielded a tuple of three arrays:

- The TPR array (denoted by `tpr`)
- The FPR array (denoted by `fpr`)
- A custom set of thresholds to calculate TPR and FPR (denoted by `ths`)

To elaborate on the **false positive rate (FPR)**, it describes the rate of false alarms. It is the number of people incorrectly thought to have diabetes although they do not:

$$FPR = \frac{\text{People incorrectly labelled having diabetes}}{\text{People who do not have diabetes}}$$

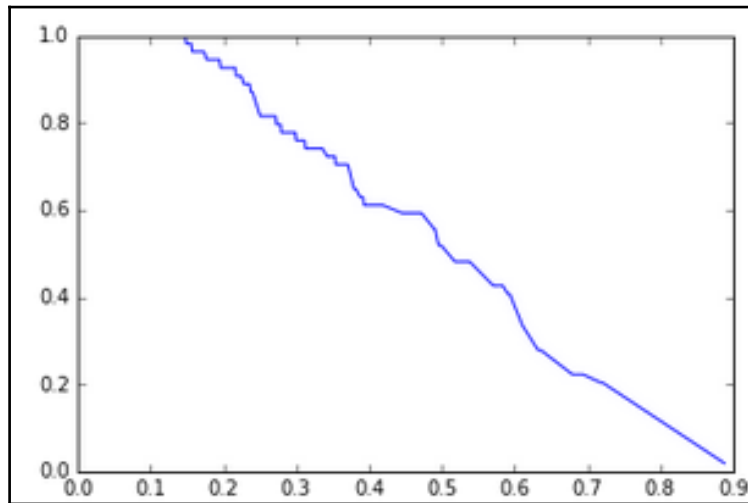
It is a statement of people who do not have diabetes. Mathematically, with the cells of the confusion matrix:

$$FPR = \frac{\text{False Positive}}{\text{False Positive} + \text{True Negative}}$$

Plotting sensitivity

2. Plot sensitivity in the y axis and the thresholds in the x axis:

```
plt.plot(ths, tpr)
```



3. Thus, the lower the threshold, the better the sensitivity. Looking at the confusion matrix for the threshold at 0.1:

```
y_pred_th= binarize(y_pred_proba, threshold=0.1)
confusion_matrix(y_test, y_pred_th[:,1], labels=[1,0])

array([[54,  0],
       [81, 19]])
```

4. In this case, no one went home believing they had diabetes when they did not. Yet, like our computation with NPV, when the test predicts that someone has diabetes, it is very inaccurate. The best scenario of this type is when the threshold is 0.146:

```
y_pred_th = binarize(y_pred_proba, threshold=0.146)
confusion_matrix(y_test, y_pred_th[:,1], labels=[1,0])

array([[54,  0],
       [67, 33]])
```

Even then, the test does not work when the person is predicted to have diabetes. It works $33 / (33 + 121) = 0.21$, or 21% of the time.

There's more...

The confusion matrix in a non-medical context

Suppose you are a banker and want to determine whether a customer deserves a mortgage loan to buy a house. Up next is a possible confusion matrix showing whether to give a person a mortgage loan based on customer data available to the bank.

The task is to classify people and determine whether they should receive a mortgage loan or not. In this context, numbers can be assigned to every scenario. When every cell in the confusion matrix has a clear cost, it is easier to find the best classifier:

		Predictions	
		LOAN AWARDED	LOAN NOT AWARDED
Truth	LOAN DESERVED	LOAN FULLY PAID	LOAN SHOULD HAVE BEEN GIVEN
	LOAN NOT DESERVED	LOAN DEFAULTS (HEAVY LOSSES)	LOAN NOT GIVEN

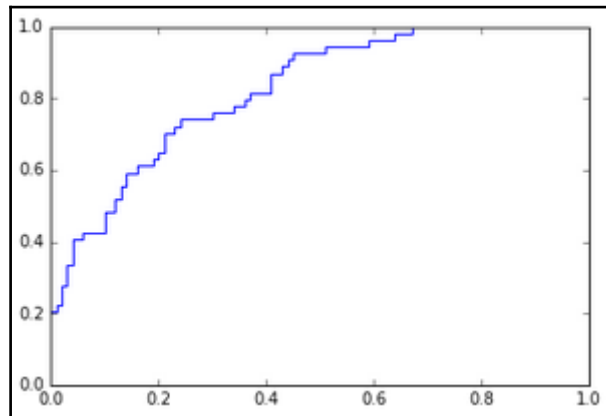
Plotting an ROC curve without context

How to do it...

An ROC curve is a diagnostic tool for any classifier without any context. No context means that we do not know yet which error type (FP or FN) is less desirable yet. Let us plot it right away using a vector of probabilities, `y_pred_proba[:,1]`:

```
from sklearn.metrics import roc_curve

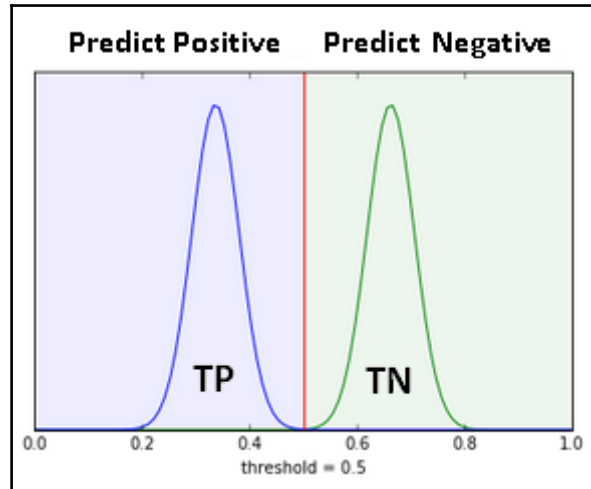
fpr, tpr, ths = roc_curve(y_test, y_pred_proba[:,1])
plt.plot(fpr, tpr)
```



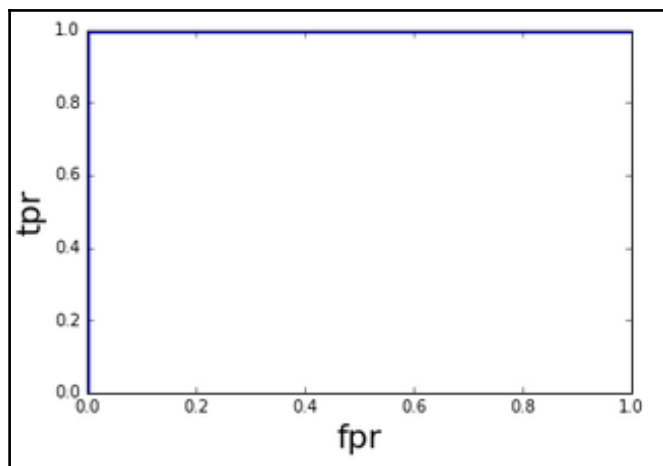
The ROC is a plot of the FPR (false alarms) in the x axis and TPR (finding everyone with the condition who really has it) in the y axis. Without context, it is a tool to measure classifier performance.

Perfect classifier

A perfect classifier would have a TPR of 1 regardless of the **false alarm rate (FAR)**:

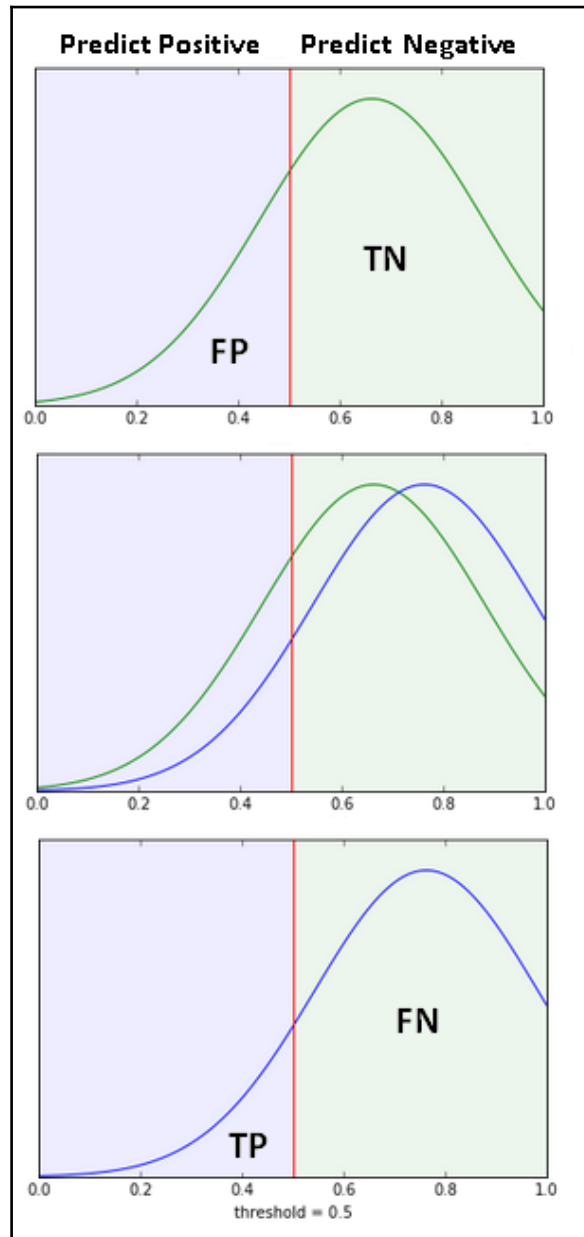


In the preceding graph, FN is very small; so the TPR, $TP / (TP + FN)$, is close to 1. Its ROC curve has an L-shape:

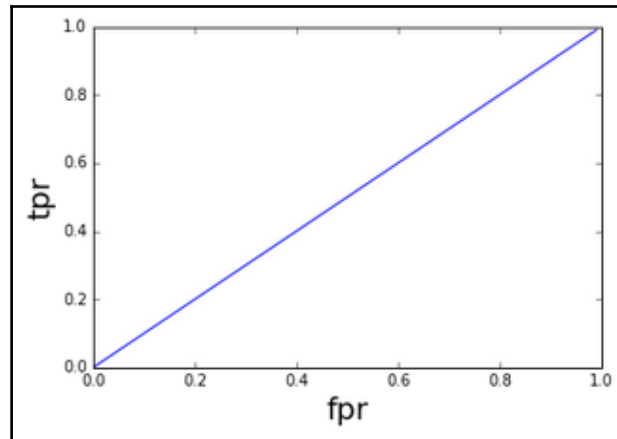


Imperfect classifier

In the following images, the distributions overlap and the categories cannot be distinguished from one another:



In the imperfect classifier, FN and TN are nearly equal and so are FP and TP. Thus, by substitution, the TPR $TP / (TP + FP)$ is nearly equal to the **false negative rate (FNR)** $FP / (FP + TN)$. This is true even if you vary the threshold. Consequently, we obtain an ROC curve that is a straight line with a slope of about 1:



AUC – the area under the ROC curve

The area of the L-shaped perfect classifier is $1 \times 1 = 1$. The area of the bad classifier is 0.5. To measure classifier performance, scikit-learn has a handy **area under the ROC curve (AUC)** calculating function:

```
from sklearn.metrics import auc

auc(fpr, tpr)

0.825185185185
```

Putting it all together – UCI breast cancer dataset

How to do it...

The dataset is provided thanks to Street, N (1990), UCI machine learning repository (<https://archive.ics.uci.edu/ml/machine-learning-databases/breast-cancer-wisconsin/breast-cancer-wisconsin.data>), Madison, WI: University of Wisconsin, computer sciences department:

1. After reading the citation/license information, load the dataset from UCI:

```
import numpy as np
import pandas as pd
data_web_address = data_web_address =
"https://archive.ics.uci.edu/ml/machine-learning-databases/breast-cancer-wisconsin/breast-cancer-wisconsin.data"
column_names = ['radius',
                'texture',
                'perimeter',
                'area',
                'smoothness',
                , 'compactness',
                'concavity',
                'concave points',
                'symmetry',
                'malignant']

feature_names = column_names[:-1]
all_data = pd.read_csv(data_web_address , names=column_names)
```

2. Look at the data types:

```
all_data.dtypes

radius          int64
texture         int64
perimeter       int64
area           int64
smoothness      int64
compactness     object
concavity       int64
concave points  int64
symmetry        int64
```

```
malignant      int64
dtype: object
```

It turns out that the feature compactness has characters like ?. For now, we do not use this feature.

- Now, reading the documentation, the target variable is set to 2 (not having cancer) and 4 (having cancer). Change the variables to 0 for not having cancer and 1 for having cancer:

```
#changing the state of having cancer to 1, not having cancer to 0
all_data['malignant'] = all_data['malignant'].astype(np.int)
all_data['malignant'] = np.where(all_data['malignant'] == 4, 1, 0)
#4, and now 1 means malignant
all_data['malignant'].value_counts()

0      458
1      241
Name: malignant, dtype: int64
```

- Define x and y :

```
X = all_data[[col for col in feature_names if col !=
'compactness']]
y = all_data.malignant
```

- Split x and y into training and testing sets:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=7, stratify=y)

#Train and test the Logistic Regression. Use the method
#predict_proba().
from sklearn.linear_model import LogisticRegression

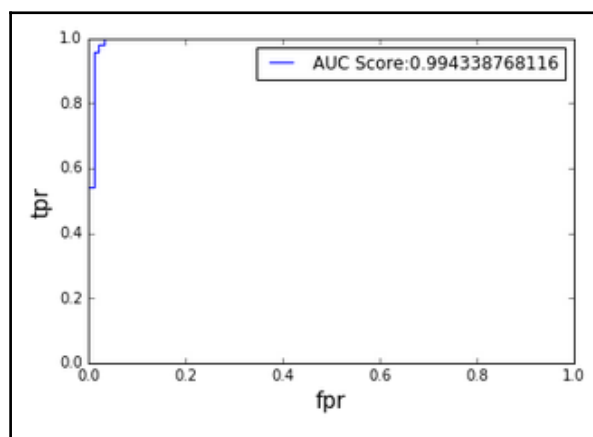
lr = LogisticRegression()
lr.fit(X_train, y_train)
y_pred_proba = lr.predict_proba(X_test)
```


6. Draw the ROC curve and compute the AUC score:

```
import matplotlib.pyplot as plt
from sklearn.metrics import roc_curve, auc, roc_auc_score

fpr, tpr, ths = roc_curve(y_test, y_pred_proba[:,1])

auc_score = auc(fpr,tpr)
plt.plot(fpr,tpr,label="AUC Score:" + str(auc_score))
plt.xlabel('fpr',fontsize='15')
plt.ylabel('tpr',fontsize='15')
plt.legend(loc='best')
```



This classifier performs fairly well.

Outline for future projects

Overall, for future classification projects, you can do the following:

1. Load the best data you can find for a particular problem.
2. Determine whether there is a classification context: is FP better or worse than FN?
3. Perform training and testing of the data without context using ROC-AUC scores.
If several algorithms perform poorly at this step, you might want to go back to step 1.
4. If the context is important, explore it with confusion matrices.

Logistic regression is particularly well suited for all these steps, though any algorithm with a `predict_proba()` method will work very similarly. As an exercise, you can generalize this process for other algorithms or even general regression if you are ambitious. The main point here is that not all errors are the same, a point easily emphasized with health datasets, wherein it is very important to treat all patients that have a condition.

A final note on the breast cancer dataset: observe that the data consists of cell measurements. You can gather these measurements by automating looking at the pictures with computers and finding the measurements with a traditional program or machine learning.

6

Building Models with Distance Metrics

This chapter will cover the following recipes:

- Using k-means to cluster data
- Optimizing the number of centroids
- Assessing cluster correctness
- Using MiniBatch k-means to handle more data
- Quantizing an image with k-means clustering
- Finding the closest objects in the feature space
- Probabilistic clustering with Gaussian Mixture Models
- Using k-means for outlier detection
- Using KNN for regression

Introduction

In this chapter, we'll cover clustering. Clustering is often grouped with unsupervised techniques. These techniques assume that we do not know the outcome variable. This leads to ambiguity in outcomes and objectives in practice, but nevertheless, clustering can be useful. As we'll see, we can use clustering to localize our estimates in a supervised setting. This is perhaps why clustering is so effective; it can handle a wide range of situations, and often the results are, for the lack of a better term, sane.

We'll walk through a wide variety of applications in this chapter, from image processing to regression and outlier detection. Clustering is related to classification of categories. You have a finite set of blobs or categories. Unlike classification, you do not know the categories in advance. Additionally, clustering can often be viewed through a continuous and probabilistic or optimization lens.

Different interpretations lead to various trade-offs. We'll walk through how to fit the models here so that you'll have the tools to try out many models when faced with a clustering problem.

Using k-means to cluster data

In a dataset, we observe sets of points gathered together. With k-means, we will categorize all the points into groups, or clusters.

Getting ready

First, let's walk through some simple clustering; then we'll talk about how k-means works:

```
import numpy as np
import pandas as pd

from sklearn.datasets import make_blobs
blobs, classes = make_blobs(500, centers=3)
```

Also, since we'll be doing some plotting, import `matplotlib` as shown:

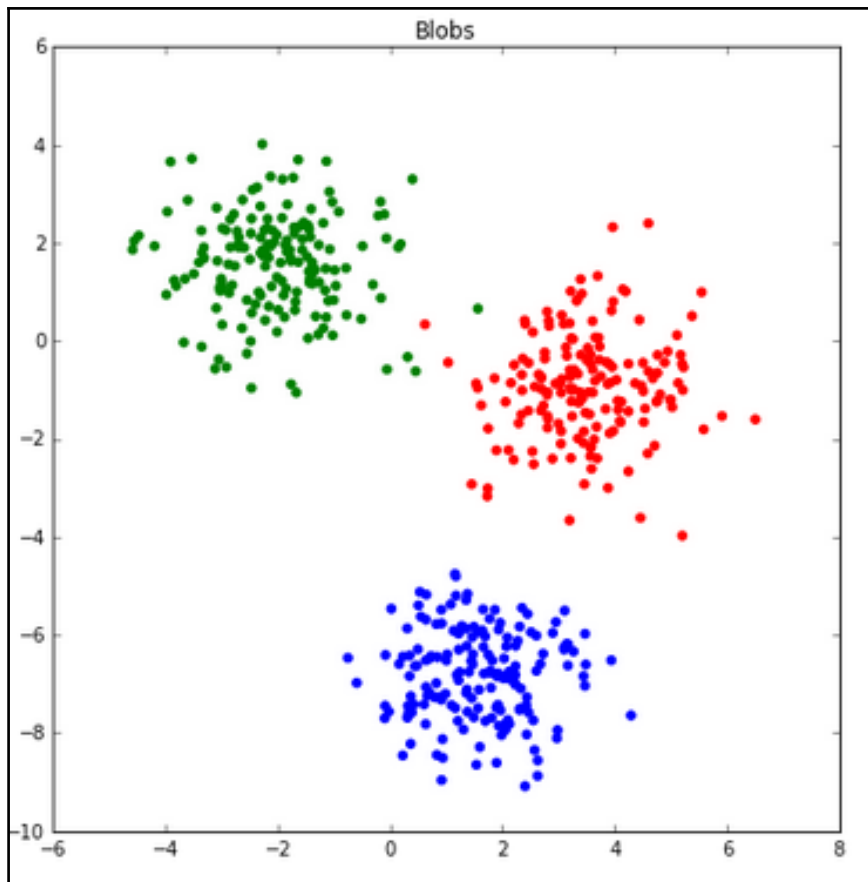
```
import matplotlib.pyplot as plt
%matplotlib inline #Within an ipython notebook
```

How to do it...

We are going to walk through a simple example that clusters blobs of fake data. Then we'll talk a little bit about how k-means works to find the optimal number of blobs:

1. Looking at our blobs, we can see that there are three distinct clusters:

```
f, ax = plt.subplots(figsize=(7.5, 7.5))
rgb = np.array(['r', 'g', 'b'])
ax.scatter(blobs[:, 0], blobs[:, 1], color=rgb[classes])
ax.set_title("Blobs")
```



Now we can use k-means to find the centers of these clusters.

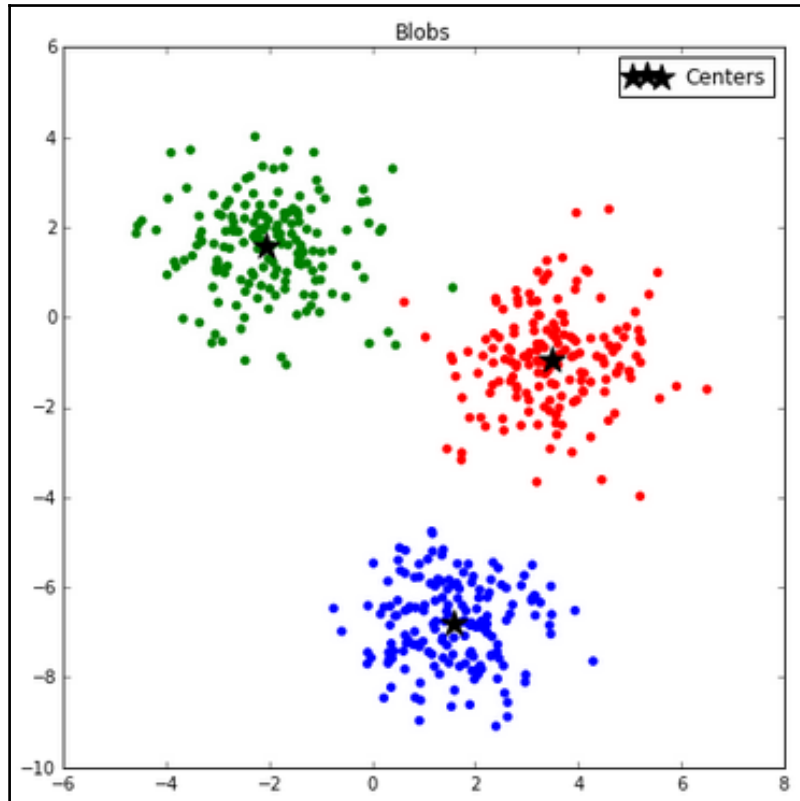
2. In the first example, we'll pretend we know that there are three centers:

```
from sklearn.cluster import KMeans
kmean = KMeans(n_clusters=3)

kmean.fit(blobs)
KMeans(algorithm='auto', copy_x=True, init='k-means++',
max_iter=300,
      n_clusters=3, n_init=10, n_jobs=1, precompute_distances='auto',
      random_state=None, tol=0.0001, verbose=0)
kmean.cluster_centers_
array([[ 3.48939154, -0.92786786],
       [-2.05114953,  1.58697731],
       [ 1.58182736, -6.80678064]])
```

```
f, ax = plt.subplots(figsize=(7.5, 7.5))
ax.scatter(blobs[:, 0], blobs[:, 1], color=rgb[classes])
ax.scatter(kmean.cluster_centers_[0], kmean.cluster_centers_[1], marker='*', s=250, color='black', label='Centers')
ax.set_title("Blobs")
ax.legend(loc='best')
```

3. The following screenshot shows the output:



4. Other attributes are useful too. For instance, the `labels_` attribute will produce the expected label for each point:

```
kmean.labels_[:5]
array([2, 0, 1, 1, 0])
```

We can check whether `kmean.labels_` is the same as the classes, but because k-means has no knowledge of the classes going in, it cannot assign the sample index values to both classes:

```
classes[:5]
array([2, 0, 1, 1, 0])
```

Feel free to swap 1 and 0 in classes to check whether it matches up with `labels_`. The transform function is quite useful in the sense that it will output the distance between each point and the centroid:

```
kmean.transform(blobs)[:5]
array([[ 6.75214231,  9.29599311,  0.71314755], [ 3.50482136,  6.7010513 ,
  9.68538042], [ 6.07460324,  1.91279125,  7.74069472], [ 6.29191797,
  0.90698131,  8.68432547], [ 2.84654338,  6.07653639,  3.64221613]])
```

How it works...

k-means is actually a very simple algorithm that works to minimize the within-cluster sum of squares of distances from the mean. We'll be minimizing the sum of squares yet again!

It does this by first setting a prespecified number of clusters, *K*, and then alternating between the following:

- Assigning each observation to the nearest cluster
- Updating each centroid by calculating the mean of each observation assigned to this cluster

This happens until some specified criterion is met. Centroids are difficult to interpret, and it can also be very difficult to determine whether we have the correct number of centroids. It's important to understand whether your data is unlabeled or not as this will directly influence the evaluation measures you can use.

Optimizing the number of centroids

When doing k-means clustering, we really do not know the right number of clusters in advance, so finding this out is an important step. Once we know (or estimate) the number of centroids, the problem will start to look more like a classification one as our knowledge to work with will have increased substantially.

Getting ready

Evaluating the model performance for unsupervised techniques is a challenge. Consequently, `sklearn` has several methods for evaluating clustering when a ground truth is known, and very few for when it isn't.

We'll start with a single cluster model and evaluate its similarity. This is more for the purpose of mechanics as measuring the similarity of one cluster count is clearly not useful in finding the ground truth number of clusters.

How to do it...

1. To get started, we'll create several blobs that can be used to simulate clusters of data:

```
from sklearn.datasets import make_blobs
import numpy as np
blobs, classes = make_blobs(500, centers=3)

from sklearn.cluster import KMeans
kmean = KMeans(n_clusters=3)
kmean.fit(blobs)
KMeans(algorithm='auto', copy_x=True, init='k-means++',
max_iter=300,
        n_clusters=3, n_init=10, n_jobs=1,
precompute_distances='auto',
        random_state=None, tol=0.0001, verbose=0)
```

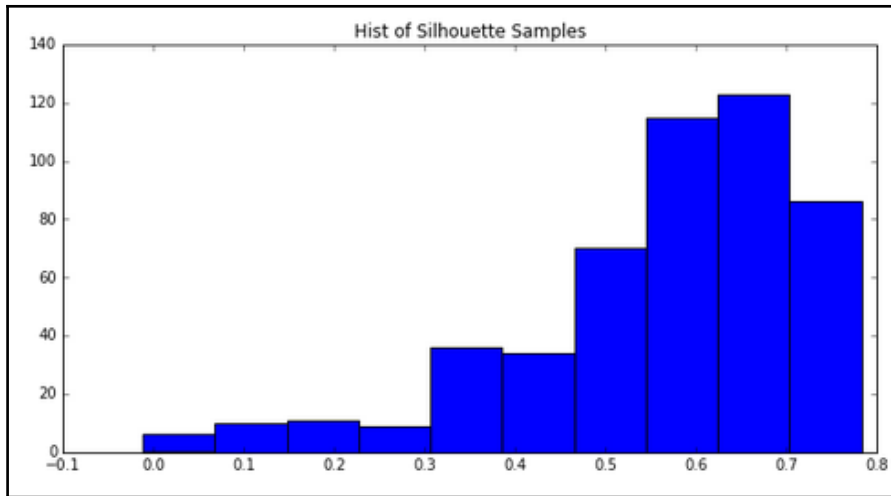
2. First, we'll look at the silhouette distance. Silhouette distance is the ratio of the difference between the in-cluster dissimilarity and the closest out-of-cluster dissimilarity, and the maximum of these two values. It can be thought of as a measure of how separate the clusters are. Let's look at the distribution of distances from the points to the cluster centers; it's useful to understand silhouette distances:

```
from sklearn import metrics
silhouette_samples = metrics.silhouette_samples(blobs,
kmean.labels_)
np.column_stack((classes[:5], silhouette_samples[:5]))
array([[ 0.          ,  0.69568017],
       [ 0.          ,  0.76789931],
       [ 0.          ,  0.62470466],
```



```
[ 0.      ,  0.6266658 ],
[ 2.      ,  0.63975981]])
```

3. The following is part of the output:



4. Notice that generally, the higher the number of coefficients close to 1 (which is good), the better the score.

How it works...

The average of the silhouette coefficients is often used to describe the entire model's fit:

```
silhouette_samples.mean()
0.5633513643546264
```

It's very common; in fact, the metrics module exposes a function to arrive at the value we just got:

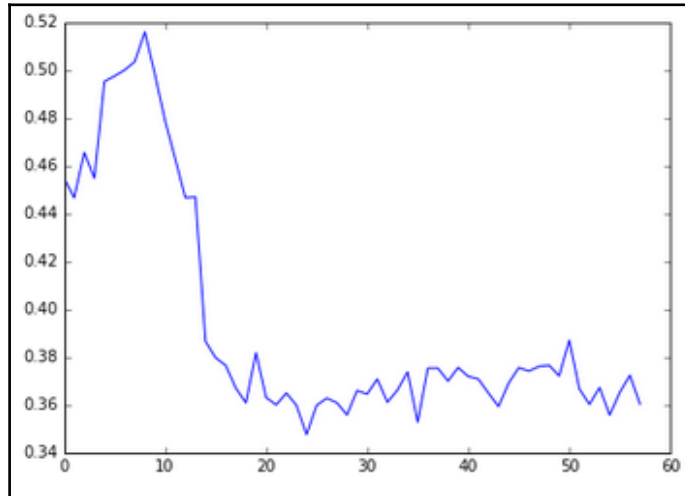
```
metrics.silhouette_score(blobs, kmean.labels_)
0.5633513643546264
import matplotlib.pyplot as plt
%matplotlib inline

blobs, classes = make_blobs(500, centers=10)
silhouette_avgs = []
for k in range(2, 60):
    kmean = KMeans(n_clusters=k).fit(blobs)
```

```
silhouette_avgs.append(metrics.silhouette_score(blobs, kmean.labels_))

f, ax = plt.subplots(figsize=(7, 5))
ax.plot(silhouette_avgs)
```

The following is the output:



This plot shows that the silhouette averages as the number of centroids increase. We can see that the optimum number, according to the data generating process, is 3; but here it looks like it's around 7 or 8. This is the reality of clustering; quite often, we won't get the correct number of clusters. We can only really hope to estimate the number of clusters to some approximation.

Assessing cluster correctness

We talked a little bit about assessing clusters when the ground truth is not known. However, we have not yet talked about assessing k-means when the cluster is known. In a lot of cases, this isn't knowable; however, if there is outside annotation, we will know the ground truth or at least the proxy sometimes.

Getting ready

So, let's assume a world where we have an outside agent supplying us with the ground truth.

We'll create a simple dataset, evaluate the measures of correctness against the ground truth in several ways, and then discuss them:

```
from sklearn import datasets
from sklearn import cluster

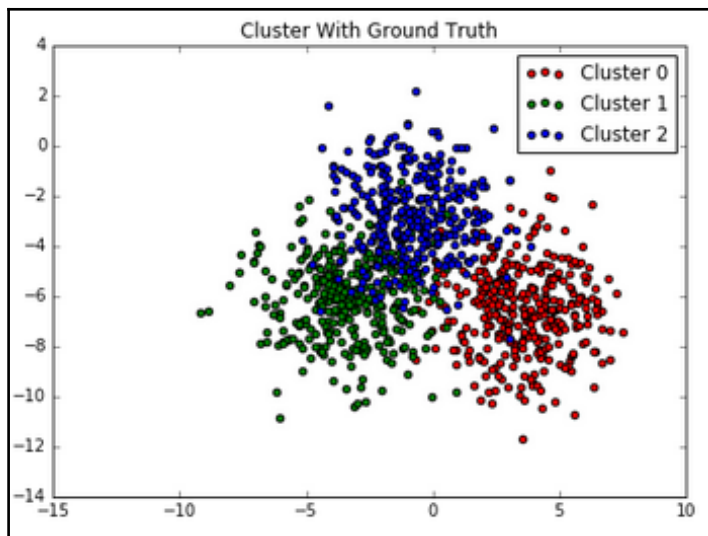
blobs, ground_truth = datasets.make_blobs(1000, centers=3, cluster_std=1.75)
```

How to do it...

1. Before we walk through the metrics, let's take a look at the dataset:

```
%matplotlib inline
import matplotlib.pyplot as plt

f, ax = plt.subplots(figsize=(7, 5))
colors = ['r', 'g', 'b']
for i in range(3):
    p = blobs[ground_truth == i]
    ax.scatter(p[:,0], p[:,1], c=colors[i],
              label="Cluster {}".format(i))
ax.set_title("Cluster With Ground Truth")
ax.legend()
```



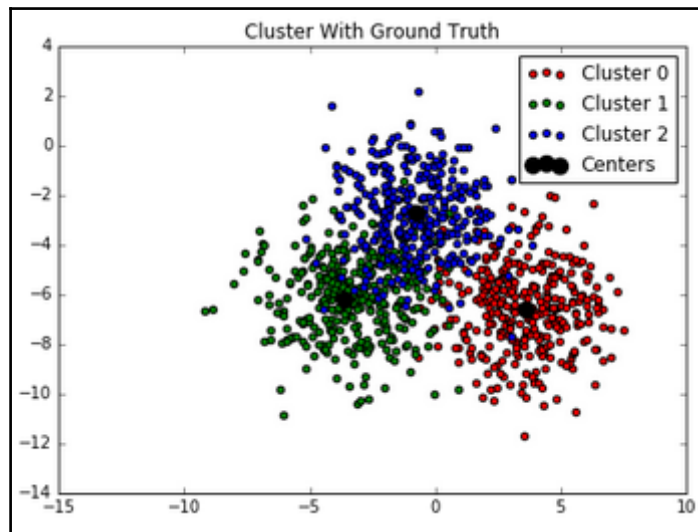
2. In order to fit a k-means model, we'll create a `KMeans` object from the cluster module:

```
kmeans = cluster.KMeans(n_clusters=3)
kmeans.fit(blobs)
KMeans(algorithm='auto', copy_x=True, init='k-means++',
max_iter=300,
        n_clusters=3, n_init=10, n_jobs=1,
precompute_distances='auto',
        random_state=None, tol=0.0001, verbose=0)
kmeans.cluster_centers_
array([[ 3.61594791, -6.6125572 ],
       [-0.76071938, -2.73916602],
       [-3.64641767, -6.23305142]])
```

3. Now that we've fit the model, let's have a look at the cluster centroids:

```
f, ax = plt.subplots(figsize=(7, 5))
colors = ['r', 'g', 'b']
for i in range(3):
    p = blobs[ground_truth == i]
    ax.scatter(p[:,0], p[:,1], c=colors[i], label="Cluster
{}".format(i))
```

The following is the output:



4. Now that we can view the clustering performance as a classification exercise, the metrics that are useful in its context are also useful here:

```
for i in range(3):
    print (kmeans.labels_ == ground_truth)[ground_truth ==
i].astype(int).mean()
0.946107784431
0.135135135135
0.0750750750751
```

Clearly, we have some backward clusters. So, let's get this straightened out first, and then we'll look at the accuracy:

```
new_ground_truth = ground_truth.copy()
new_ground_truth[ground_truth == 1] = 2
new_ground_truth[ground_truth == 2] = 1
0.946107784431
0.852852852853
0.891891891892
```

So, we're roughly correct 90% of the time. The second measure of similarity we'll look at is the mutual information score:

```
from sklearn import metrics
metrics.normalized_mutual_info_score(ground_truth, kmeans.labels_)
0.66467613668253844
```

As the score tends to be 0, the label assignments are probably not generated through similar processes; however, a score closer to 1 means that there is a large amount of agreement between the two labels.

For example, let's look at what happens when the mutual information score itself:

```
metrics.normalized_mutual_info_score(ground_truth, ground_truth)
1.0
```

Given the name, we can tell that there is probably an unnormalized `mutual_info_score`:

```
metrics.mutual_info_score(ground_truth, kmeans.labels_)
0.72971342940406325
```

These are very close; however, normalized mutual information is the mutual information divided by the root of the product of the entropy of each set truth and assigned label.

There's more...

One cluster metric we haven't talked about yet, and one that is not reliant on the ground truth, is inertia. It is not very well documented as a metric at the moment. However, it is a metric that k-means minimizes.

Inertia is the sum of the squared difference between each point and its assigned cluster. We can use a bite of NumPy to determine this:

```
kmeans.inertia_  
4849.9842988128385
```

Using MiniBatch k-means to handle more data

K-means is a nice method to use; however, it is not ideal for a lot of data. This is due to the complexity of k-means. This said, we can get approximate solutions with much better algorithmic complexity using MiniBatch k-means.

Getting ready

MiniBatch k-means is a faster implementation of k-means. K-means is computationally very expensive; the problem is NP-hard.

However, using MiniBatch k-means, we can speed up k-means by orders of magnitude. This is achieved by taking many subsamples that are called MiniBatches. Given the convergence properties of subsampling, a close approximation to regular k-means is achieved provided there are good initial conditions.

How to do it...

1. Let's do some very high-level profiling of MiniBatch clustering. First, we'll look at the overall speed difference, and then we'll look at the errors in the estimates:

```
import numpy as np  
from sklearn.datasets import make_blobs  
blobs, labels = make_blobs(int(1e6), 3)  
  
from sklearn.cluster import KMeans, MiniBatchKMeans
```

```
kmeans = KMeans(n_clusters=3)
minibatch = MiniBatchKMeans(n_clusters=3)
```



Understand that these metrics are meant to expose the issue. Therefore, great care is taken to ensure the highest accuracy of the benchmarks. There is a lot of information available on this topic; if you really want to get to the heart of why MiniBatch k-means is better at scaling, it will be a good idea to review what's available.

2. Now that the setup is complete, we can measure the time difference:

```
%time kmeans.fit(blobs) #IPython Magic
Wall time: 7.88 s

KMeans(algorithm='auto', copy_x=True, init='k-means++',
max_iter=300,
      n_clusters=3, n_init=10, n_jobs=1, precompute_distances='auto',
      random_state=None, tol=0.0001, verbose=0)
%time minibatch.fit(blobs)
Wall time: 2.66 s

MiniBatchKMeans(batch_size=100, compute_labels=True, init='k-
means++',
      init_size=None, max_iter=100, max_no_improvement=10,
n_clusters=3,
      n_init=3, random_state=None, reassignment_ratio=0.01,
tol=0.0,
      verbose=0)
```

3. There's a large difference in CPU times. The difference in the clustering performance is shown as follows:

```
kmeans.cluster_centers_
array([[ -3.74304286, -0.4289715 , -8.69684375],
       [-5.73689621, -6.39166391,  6.18598804],
       [ 0.63866644, -9.93289824,  3.24425045]])
minibatch.cluster_centers_
array([[ -3.72580548, -0.46135647, -8.63339789],
       [-5.67140979, -6.33603949,  6.21512625],
       [ 0.64819477, -9.87197712,  3.26697532]])
```

4. Look at the two arrays; the located centers are ordered the same. This is random—the clusters do not have to be ordered the same. Look at the distance between the first cluster centers:

```
from sklearn.metrics import pairwise
pairwise.pairwise_distances(kmeans.cluster_centers_[0].reshape(1,
-1), minibatch.cluster_centers_[0].reshape(1, -1))
array([[ 0.07328909]])
```

5. This seems to be very close. The diagonals will contain the cluster center differences:

```
np.diag(pairwise.pairwise_distances(kmeans.cluster_centers_,
minibatch.cluster_centers_))
array([ 0.07328909,  0.09072807,  0.06571599])
```

How it works...

The batches here are key. Batches are iterated through to find the batch mean; for the next iteration, the prior batch mean is updated in relation to the current iteration. There are several options that dictate the general k-means behavior and parameters that determine how MiniBatch k-means gets updated.

The `batch_size` parameter determines how large the batches should be. Just for fun, let's run MiniBatch; however, this time we set the batch size to be the same as the dataset size:

```
minibatch = MiniBatchKMeans(batch_size=len(blobs))
%time minibatch.fit(blobs)
Wall time: 1min

MiniBatchKMeans(batch_size=1000000, compute_labels=True, init='k-means++',
init_size=None, max_iter=100, max_no_improvement=10, n_clusters=8,
n_init=3, random_state=None, reassignment_ratio=0.01, tol=0.0,
verbose=0)
```

Clearly, this is against the spirit of the problem, but it does illustrate an important point. Choosing poor initial conditions can affect how well models, particularly clustering models, converge. With MiniBatch k-means, there is no guarantee that the global optimum will be achieved.

There are many powerful lessons in MiniBatch k-means. It uses the power of many random samples, similar to bootstrapping. When creating an algorithm for big data, you can use many random samples on many machines processing in parallel.

Quantizing an image with k-means clustering

Image processing is an important topic in which clustering has some application. It's worth pointing out that there are several very good image processing libraries in Python. `scikit-image` is a sister project of `scikit-learn`. It's worth taking a look at if you want to do anything complicated.

A big point of this chapter is that images are data as well and clustering can be used to try to guess where some objects in an image are. Clustering can be part of an image processing pipeline.

Getting ready

We will have some fun in this recipe. The goal is to use a cluster to blur an image. First, we'll make use of SciPy to read the image. The image is translated in a three-dimensional array; the `x` and `y` coordinates describe the height and width, and the third dimension represents the RGB values for each image.

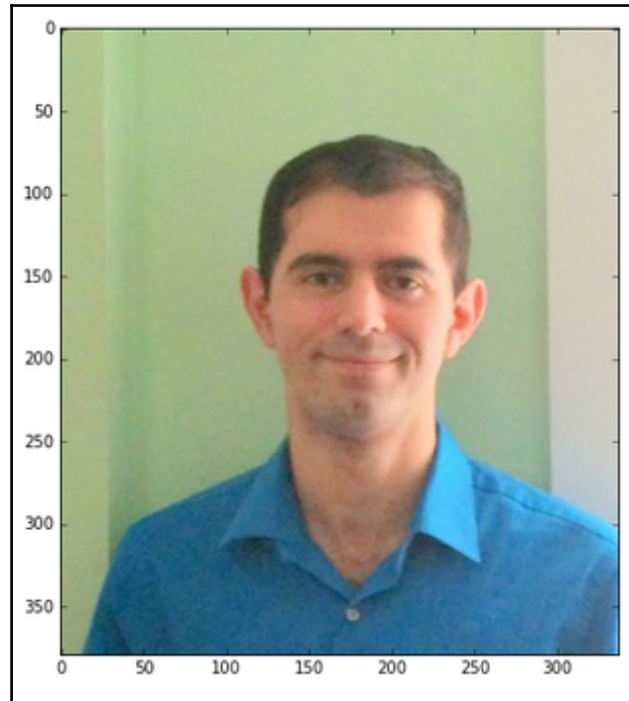
Begin by downloading or moving an `.jpg` image to the folder where your IPython notebook is located. You can use a picture of yours. I use a picture of myself named `headshot.jpg`.

How do it...

1. Now, let's read the image in Python:

```
%matplotlib inline
import matplotlib.pyplot as plt
from scipy import ndimage
img = ndimage.imread("headshot.jpg")
plt.figure(figsize = (10,7))
plt.imshow(img)
```

The following image is seen:



2. That's me! Now that we have the image, let's check its dimensions:

```
img.shape  
(379L, 337L, 3L)
```

To actually quantize the image, we need to convert it into a two-dimensional array, with the length being 379×337 and the width being the RGB values. A better way to think about this is to have a bunch of data points in three-dimensional space and cluster the points to reduce the number of distant colors in the image—a simple way to do quantization.

3. First, let's reshape our array; it is a NumPy array, and thus simple to work with:

```
x, y, z = img.shape
long_img = img.reshape(x*y, z)
long_img.shape
(127723L, 3L)
```

4. Now we can start the clustering process. First, let's import the cluster module and create a k-means object. We'll pass `n_clusters=5` so that we have five clusters, or really, five distinct colors. This will be a good recipe to practice using silhouette distance, which we reviewed in the *Optimizing the number of centroids* recipe:

```
from sklearn import cluster
k_means = cluster.KMeans(n_clusters=5)
k_means.fit(long_img)
centers = k_means.cluster_centers_
centers
array([[ 169.01964615,  123.08399844,   99.6097561 ],
       [  45.79271071,   94.56844879,  120.00911162],
       [ 218.74043562,  202.152748 ,  184.14355039],
       [  67.51082485,  151.50671141,  201.9408963 ],
       [ 169.69235986,  189.63274724,  143.75511521]])
```

How it works...

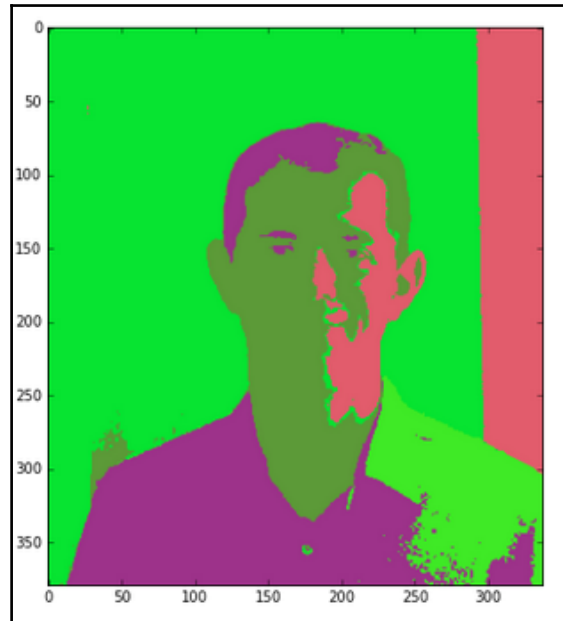
Now that we have the centers, the next thing we need is the labels. This will tell us which points should be associated with which clusters:

```
labels = k_means.labels_
labels
array([4, 4, 4, ..., 3, 3, 3])
```

At this point, we require the simplest of NumPy array manipulation followed by a bit of reshaping, and we'll have the new image:

```
plt.figure(figsize = (10,7))
plt.imshow(centers[labels].reshape(x, y, z))
```

The following is the resultant image:



The clustering separated the image into a few regions.

Finding the closest object in the feature space

Sometimes, the easiest thing to do is to find the distance between two objects. We just need to find some distance metric, compute the pairwise distances, and compare the outcomes with what is expected.

Getting ready

A lower level utility in scikit-learn is `sklearn.metrics.pairwise`. It contains server functions used to compute distances between vectors in a matrix `X` or between vectors in `X` and `Y` easily. This can be useful for information retrieval. For example, given a set of customers with attributes of `X`, we might want to take a reference customer and find the closest customers to this customer.

In fact, we might want to rank customers by the notion of similarity measured by a distance function. The quality of similarity depends upon the feature space selection as well as any transformation we might do on the space. We'll walk through several different scenarios of measuring distance.

How to do it...

We will use the `pairwise_distances` function to determine the closeness of objects. Remember that the closeness is just similarity, which we grade using our distance function:

1. First, let's import the pairwise distance function from the metrics module and create a dataset to play with:

```
import numpy as np

from sklearn.metrics import pairwise
from sklearn.datasets import make_blobs
points, labels = make_blobs()
```

2. The simplest way to check the distances is `pairwise_distances`:

```
distances = pairwise.pairwise_distances(points)

distances is an N x N matrix with 0s along the diagonals. In the simplest
case, let's see the distances between each point and the first point:

np.diag(distances) [:5]
distances[0] [:5]
array([ 0. , 4.24926332, 8.8630893 , 5.01378992, 10.05620093])
```

3. Ranking the points by closeness is very easy with `np.argsort`:

```
ranks = np.argsort(distances[0])
ranks[:5]
array([ 0, 63, 6, 21, 17], dtype=int64)
```

4. The great thing about `argsort` is that now we can sort our `points` matrix to get the actual points:

```
points[ranks] [:5]
array([[ -0.15728042,  -5.76309092],
       [ -0.20720885,  -5.52734277],
       [ -0.08686778,  -6.42054076],
       [  0.33493582,  -6.29824601],
       [ -0.89842683,  -5.78335127]])
```

```
sp_points = points[ranks][:5]
```

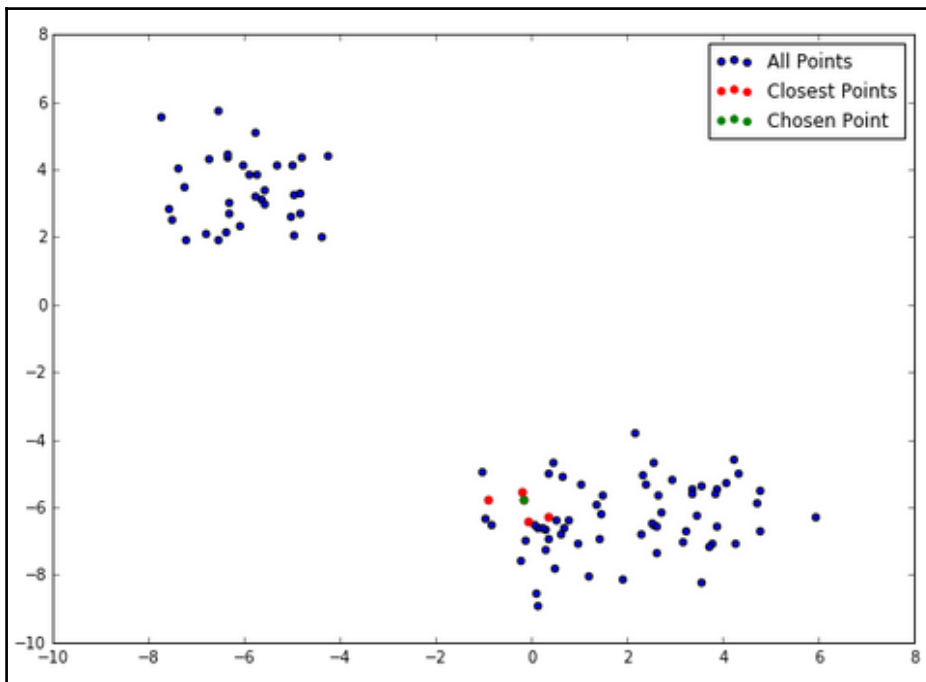
5. It's useful to see what the closest points look like as follows. The chosen point, `points[0]`, is colored green. The closest points are colored red (except for the chosen point).

Note that other than some assurances, this works as intended:

```
import matplotlib.pyplot as plt
%matplotlib inline

plt.figure(figsize=(10,7))
plt.scatter(points[:,0], points[:,1], label = 'All Points')
plt.scatter(sp_points[:,0], sp_points[:,1], color='red',
            label='Closest Points')
plt.scatter(points[0,0], points[0,1], color='green', label = 'Chosen
Point')

plt.legend()
```



How it works...

Given some distance function, each point is measured in a pairwise function. Consider two points represented as vectors in N-dimensional space with components p_i and q_i ; the default is the Euclidean distance, which is as follows:

$$d(p, q) = \sqrt{\sum_{n=1}^N (p_i - q_i)^2}$$

Verbally, this takes the difference between each component of the two vectors, squares these differences, sums them all, and then finds the square root. This looks very familiar as we used something very similar when looking at the mean squared error. If we take the square root, we have the same thing. In fact, a metric used often is root mean square deviation (RMSE), which is just the applied distance function.

In Python, this looks like the following:

```
def euclid_distances(x, y):
    return np.power(np.power(x - y, 2).sum(), .5)
euclid_distances(points[0], points[1])
4.249263322917467
```

There are several other functions available in scikit-learn, but scikit-learn will also use distance functions of SciPy. At the time of writing this book, the scikit-learn distance functions support sparse matrixes. Check out the SciPy documentation for more information on the distance functions:

- cityblock
- cosine
- euclidean
- l1
- l2
- manhattan

We can now solve problems. For example, if we were standing on a grid at the origin and the lines were the streets, how far would we have to travel to get to point (5, 5)?

```
pairwise.pairwise_distances([[0, 0], [5, 5]], metric='cityblock')[0]
array([ 0., 10.] )
```

There's more...

Using pairwise distances, we can find the similarity between bit vectors. For N-dimensional vectors p and q , it's a matter of finding the hamming distance, which is defined as follows:

$$d(p, q) = \sum_{n=1}^N I_{p_i \neq q_i}$$

Use the following command:

```
X = np.random.binomial(1, .5, size=(2, 4)).astype(np.bool)
X
array([[False, False, False, False],
       [False, True, True, True]], dtype=bool)
pairwise.pairwise_distances(X, metric='hamming')
array([[ 0. ,  0.75],
       [ 0.75,  0. ]])
```

Note that scikit-learn's `hamming` metric returns the hamming distance divided by the length of the vectors, 4 in this case.

Probabilistic clustering with Gaussian mixture models

In k-means, we assume that the variance of the clusters is equal. This leads to a subdivision of space that determines how the clusters are assigned; but what about a situation where the variances are not equal and each cluster point has some probabilistic association with it?

Getting ready

There's a more probabilistic way of looking at k-means clustering. Hard k-means clustering is the same as applying a Gaussian mixture model with a covariance matrix, S , which can be factored to the error times of the identity matrix. This is the same covariance structure for each cluster. It leads to spherical clusters. However, if we allow S to vary, a GMM can be estimated and used for prediction. We'll look at how this works in a univariate sense and then expand to more dimensions.

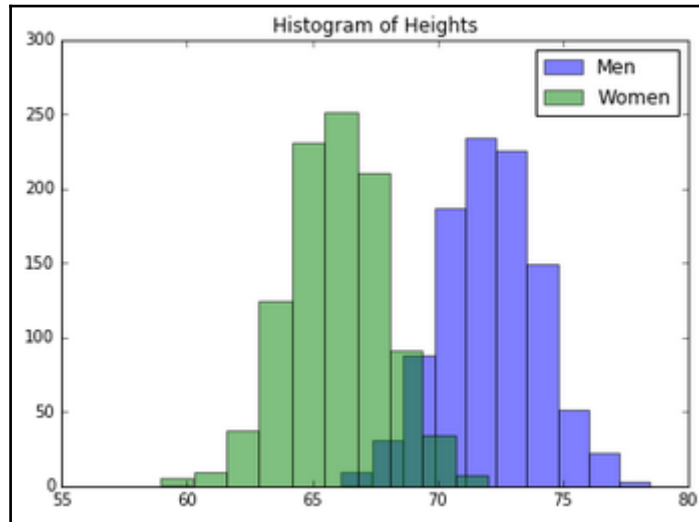
How to do it...

1. First, we need to create some data. For example, let's simulate heights of both women and men. We'll use this example throughout this recipe. It's a simple example, but hopefully it will illustrate what we're trying to accomplish in an N-dimensional space, which is a little easier to visualize:

```
import numpy as np

N = 1000
in_m = 72
in_w = 66
s_m = 2
s_w = s_m
m = np.random.normal(in_m, s_m, N)
w = np.random.normal(in_w, s_w, N)
from matplotlib import pyplot as plt
%matplotlib inline
f, ax = plt.subplots(figsize=(7, 5))
ax.set_title("Histogram of Heights")
ax.hist(m, alpha=.5, label="Men");
ax.hist(w, alpha=.5, label="Women");
ax.legend()
```

This is the output:



2. Next, we might be interested in subsampling the group, fitting the distribution, and then predicting the remaining groups:

```
random_sample = np.random.choice([True, False], size=m.size)
m_test = m[random_sample]
m_train = m[~random_sample]
w_test = w[random_sample]
w_train = w[~random_sample]
```

3. Now we need to get the empirical distribution of the heights of both men and women based on the training set:

```
from scipy import stats
m_pdf = stats.norm(m_train.mean(), m_train.std())
w_pdf = stats.norm(w_train.mean(), w_train.std())
```

For the test set, we will calculate based on the likelihood that the data point was generated from either distribution, and the most likely distribution will get the appropriate label assigned.

4. We will, of course, look at how accurate we were:

```
m_pdf.pdf(m[0])
0.19762291119664221
w_pdf.pdf(m[0])
0.00085042279862613103
```

5. Notice the difference in likelihoods. Assume that we guess situations when the men's probability is higher, but we overwrite them if the women's probability is higher:

```
guesses_m = np.ones_like(m_test)
guesses_m[m_pdf.pdf(m_test) < w_pdf.pdf(m_test)] = 0
```

6. Obviously, the question is how accurate we are. Since `guesses_m` will be 1 if we are correct and 0 if we aren't, we take the mean of the vector and get the accuracy:

```
guesses_m.mean()
0.94176706827309242
```

7. Not too bad! Now, to see how well we did with the women's group, we use the following commands:

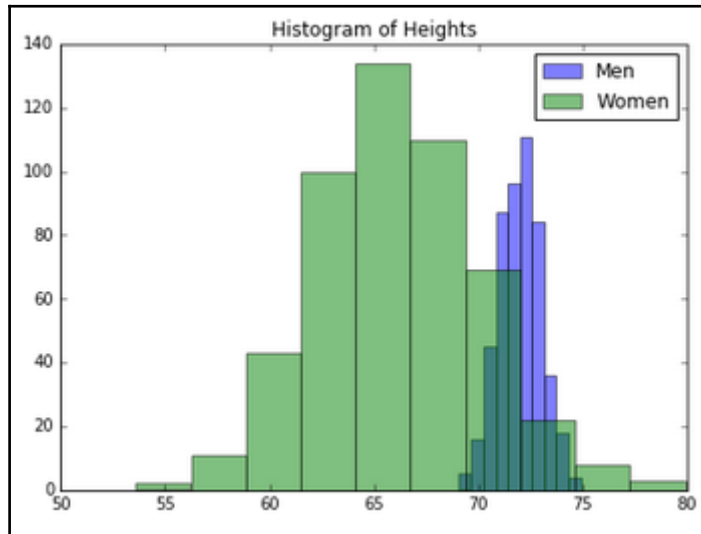
```
guesses_w = np.ones_like(w_test)
guesses_w[m_pdf.pdf(w_test) > w_pdf.pdf(w_test)] = 0
guesses_w.mean()
0.93775100401606426
```

8. Let's allow the variance to differ between groups. First, create some new data:

```
s_m = 1
s_w = 4
m = np.random.normal(in_m, s_m, N)
w = np.random.normal(in_w, s_w, N)
```

9. Then, create a training set:

```
m_test = m[random_sample]
m_train = m[~random_sample]
w_test = w[random_sample]
w_train = w[~random_sample]
f, ax = plt.subplots(figsize=(7, 5))
ax.set_title("Histogram of Heights")
ax.hist(m_train, alpha=.5, label="Men");
ax.hist(w_train, alpha=.5, label="Women");
ax.legend()
```

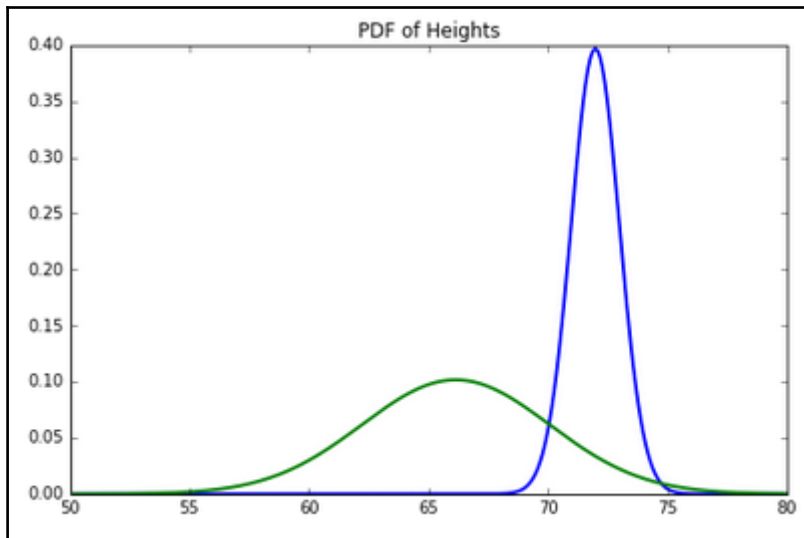


10. Now we can create the same PDFs:

```
m_pdf = stats.norm(m_train.mean(), m_train.std())
w_pdf = stats.norm(w_train.mean(), w_train.std())

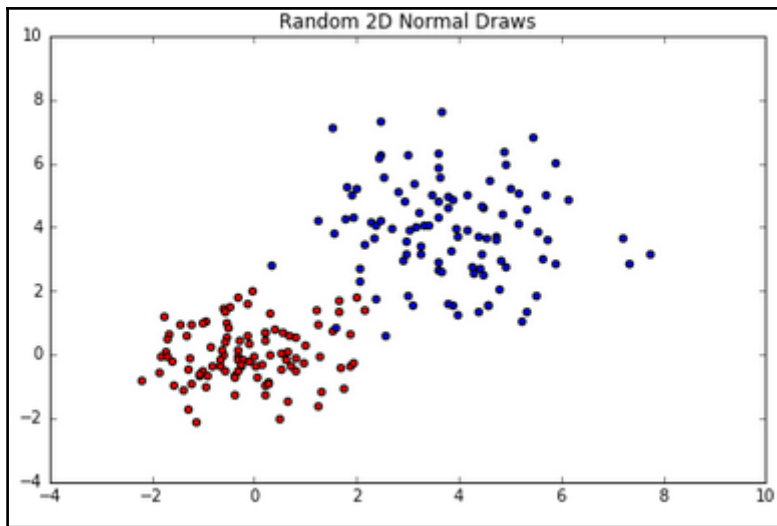
x = np.linspace(50, 80, 300)
plt.figure(figsize=(8, 5))
plt.title('PDF of Heights')
plt.plot(x, m_pdf.pdf(x), 'k', linewidth=2, color='blue',
label='Men')
plt.plot(x, w_pdf.pdf(x), 'k', linewidth=2,
color='green', label='Women')
```

11. The following is the output:



You can imagine this in a multidimensional space:

```
class_A = np.random.normal(0, 1, size=(100, 2))
class_B = np.random.normal(4, 1.5, size=(100, 2))
f, ax = plt.subplots(figsize=(8, 5))
plt.title('Random 2D Normal Draws')
ax.scatter(class_A[:,0], class_A[:,1], label='A', c='r')
ax.scatter(class_B[:,0], class_B[:,1], label='B')
```



How it works...

Okay, so now that we've looked at how we can classify points based on distribution, let's look at how we can do this in scikit-learn:

```
from sklearn.mixture import GaussianMixture
gmm = GaussianMixture(n_components=2)
X = np.row_stack((class_A, class_B))
y = np.hstack((np.ones(100), np.zeros(100)))
```

Since we're conscientious data scientists, we'll create a training set:

```
train = np.random.choice([True, False], 200)
gmm.fit(X[train])
GaussianMixture(covariance_type='full', init_params='kmeans', max_iter=100,
                 means_init=None, n_components=2, n_init=1, precisions_init=None,
                 random_state=None, reg_covar=1e-06, tol=0.001, verbose=0,
                 verbose_interval=10, warm_start=False, weights_init=None)
```

Fitting and predicting is done in the same way as fitting is done for many of the other objects in scikit-learn:

```
gmm.fit(X[train])
gmm.predict(X[train])[:5]
array([0, 0, 0, 0, 0], dtype=int64)
```

There are other methods worth looking at now that the model has been fit. For example, using `score_samples`, we can actually get the per-sample likelihood for each label.

Using k-means for outlier detection

In this recipe, we'll look at both the debate and mechanics of k-means for outlier detection. It can be useful to isolate some types of errors, but care should be taken when using it.

Getting ready

We'll use k-means to do outlier detection on a cluster of points. It's important to note that there are many camps when it comes to outliers and outlier detection. On one hand, we're potentially removing points that were generated by the data-generating process by removing outliers. On the other hand, outliers can be due to a measurement error or some other outside factor.

This is the most credence we'll give to the debate. The rest of this recipe is about finding outliers; we'll work under the assumption that our choice to remove outliers is justified. The act of outlier detection is a matter of finding the centroids of the clusters and then identifying points that are potential outliers by their distances from the centroid.

How to do it...

1. First, we'll generate a single blob of 100 points, and then we'll identify the five points that are furthest from the centroid. These are the potential outliers:

```
from sklearn.datasets import make_blobs
X, labels = make_blobs(100, centers=1)
import numpy as np
```

2. It's important that the k-means cluster has a single center. This idea is similar to a one-class SVM that is used for outlier detection:

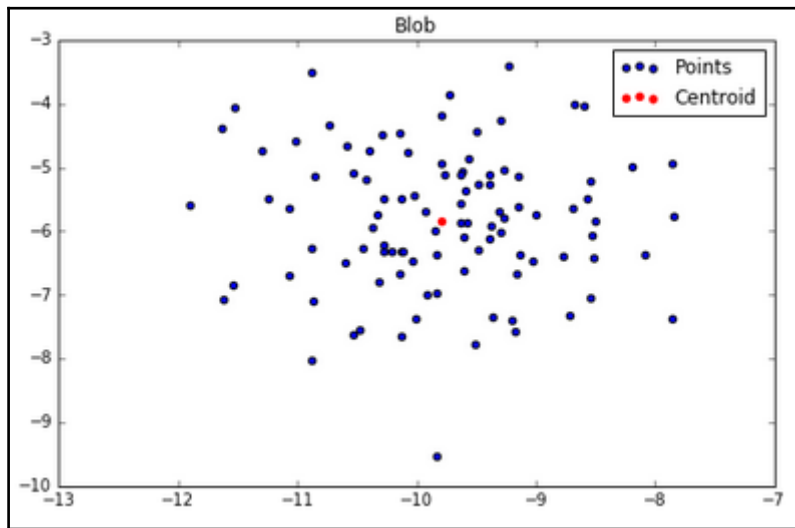
```
from sklearn.cluster import KMeans
kmeans = KMeans(n_clusters=1)
kmeans.fit(X)
KMeans(algorithm='auto', copy_x=True, init='k-means++',
max_iter=300,
n_clusters=1, n_init=10, n_jobs=1, precompute_distances='auto',
random_state=None, tol=0.0001, verbose=0)
```

3. Now, let's look at the plot. Those playing along at home, try to guess which points will be identified as one of the five outliers:

```
import matplotlib.pyplot as plt
%matplotlib inline

f, ax = plt.subplots(figsize=(8, 5))
ax.set_title("Blob")
ax.scatter(X[:, 0], X[:, 1], label='Points')
ax.scatter(kmeans.cluster_centers_[0], kmeans.cluster_centers_[1], label='Centroid', color='r')
ax.legend()
```

The following is the output:



4. Now, let's identify the five closest points:

```
distances = kmeans.transform(X)

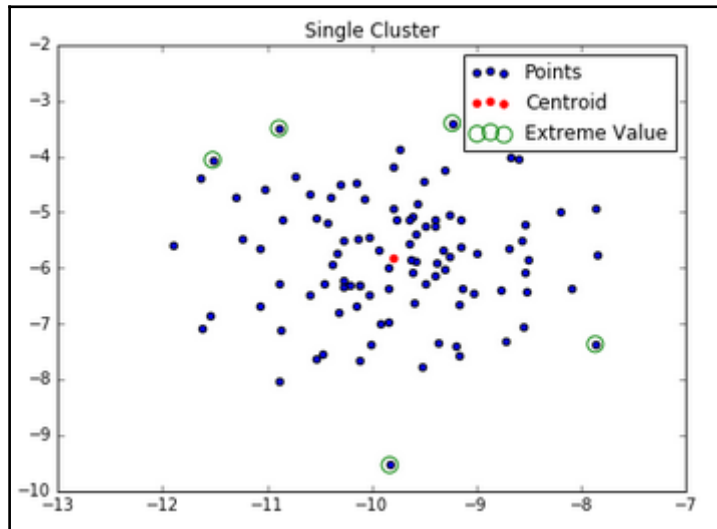
# argsort returns an array of indexes which will sort the array in
# ascending order
# so we reverse it via[::-1] and take the top five with [:5]

sorted_idx = np.argsort(distances.ravel())[::-1][:5]
```

5. Let's see which plots are the farthest away:

```
f, ax = plt.subplots(figsize=(7, 5))
ax.set_title("Single Cluster")
ax.scatter(X[:, 0], X[:, 1], label='Points')
ax.scatter(kmeans.cluster_centers_[0], kmeans.cluster_centers_[0], label='Centroid', color='r')
ax.scatter(X[sorted_idx][:, 0], X[sorted_idx][:, 1], label='Extreme Value', edgecolors='g', facecolors='none', s=100)
ax.legend(loc='best')
```

The following is the output:



6. It's easy to remove these points if we like:

```
new_X = np.delete(X, sorted_idx, axis=0)
```

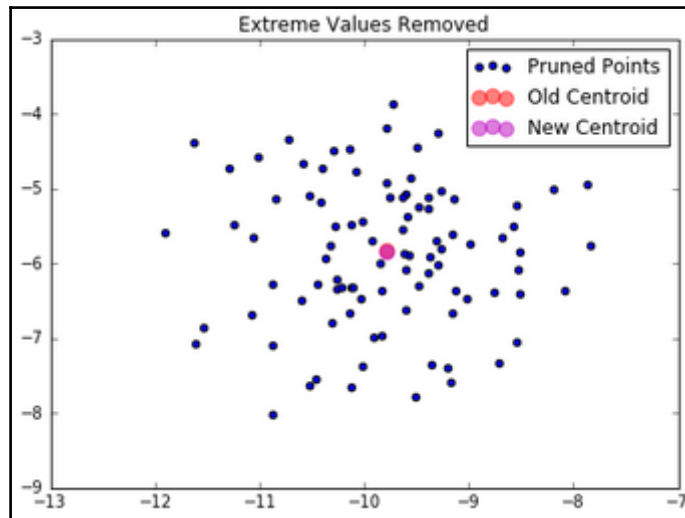
Also, the centroid clearly changes with the removal of these points:

```
new_kmeans = KMeans(n_clusters=1)
new_kmeans.fit(new_X)
```


7. Let's visualize the difference between the old and new centroids:

```
f, ax = plt.subplots(figsize=(7, 5))
ax.set_title("Extreme Values Removed")
ax.scatter(new_X[:, 0], new_X[:, 1], label='Pruned Points')
ax.scatter(kmeans.cluster_centers_[0], kmeans.cluster_centers_[0],
           label='Old Centroid', color='r', s=80, alpha=.5)
ax.scatter(new_kmeans.cluster_centers_[0], new_kmeans.cluster_centers_[0],
           label='New Centroid', color='m', s=80, alpha=.5)
ax.legend(loc='best')
```

The following is the output:



Clearly, the centroid hasn't moved much, which is to be expected only when removing the five most extreme values. This process can be repeated until we're satisfied that the data is representative of the process.

How it works...

As we've already seen, there is a fundamental connection between the Gaussian distribution and the k-means clustering. Let's create an empirical Gaussian based on the centroid and sample covariance matrix and look at the probability of each point—theoretically, the five points we removed. This just shows that we have, in fact, removed the values with the least likelihood. This idea between distances and likelihoods is very important and will come around quite often in your machine learning training. Use the following command to create an empirical Gaussian:

```
from scipy import stats
emp_dist = stats.multivariate_normal(kmeans.cluster_centers_.ravel())
lowest_prob_idx = np.argsort(emp_dist.pdf(X))[:5]
np.all(X[sorted_idx] == X[lowest_prob_idx])

True
```

Using KNN for regression

Regression is covered elsewhere in the book, but we might also want to run a regression on pockets of the feature space. We can think that our dataset is subject to several data processes. If this is true, only training on similar data points is a good idea.

Getting ready

Our old friend, regression, can be used in the context of clustering. Regression is obviously a supervised technique, so we'll use **K-Nearest Neighbors (KNN)** clustering rather than k-means. For KNN regression, we'll use the K closest points in the feature space to build the regression rather than using the entire space as in regular regression.

How to do it...

For this recipe, we'll use the `iris` dataset. If we want to predict something such as the petal width for each flower, clustering by iris species can potentially give us better results. The KNN regression won't cluster by the species, but we'll work under the assumption that the Xs will be close for the same species, in this case, the petal length:

1. We'll use the `iris` dataset for this recipe:

```
import numpy as np
from sklearn import datasets
iris = datasets.load_iris()
iris.feature_names
```

2. We'll try to predict the petal length based on the sepal length and width. We'll also fit a regular linear regression to see how well the KNN regression does in comparison:

```
X = iris.data[:, :2]
y = iris.data[:, 2]

from sklearn.linear_model import LinearRegression
lr = LinearRegression()
lr.fit(X, y)
print "The MSE is: {:.2}".format(np.power(y -
lr.predict(X), 2).mean())
```

The MSE is: 0.41

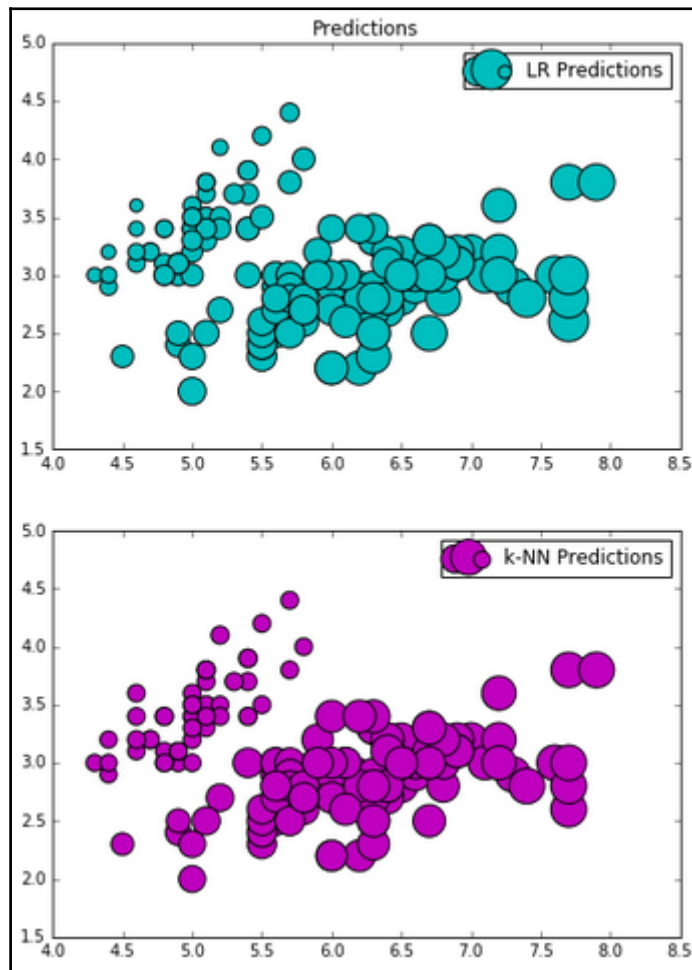
3. Now, for the KNN regression, use the following code:

```
from sklearn.neighbors import KNeighborsRegressor
knnr = KNeighborsRegressor(n_neighbors=10)
knnr.fit(X, y)
print "The MSE is: {:.2}".format(np.power(y -
knnr.predict(X), 2).mean())
```

The MSE is: 0.17

4. Let's look at what the KNN regression does when we tell it to use the 10 closest points for regression:

```
f, ax = plt.subplots(nrows=2, figsize=(7, 10))
ax[0].set_title("Predictions")
ax[0].scatter(X[:, 0], X[:, 1], s=lr.predict(X)*80, label='LR
Predictions', color='c', edgecolors='black')
ax[1].scatter(X[:, 0], X[:, 1], s=knnr.predict(X)*80, label='k-NN
Predictions', color='m', edgecolors='black')
ax[0].legend()
ax[1].legend()
```



5. It might be completely clear that the predictions are close for the most part, but let's look at the predictions for the Setosa species as compared to the actuals:

```
setosa_idx = np.where(iris.target_names=='setosa')
setosa_mask = iris.target == setosa_idx[0]
y[setosa_mask][:5]
array([ 1.4,  1.4,  1.3,  1.5,  1.4])
knnr.predict(X)[setosa_mask][:5]
array([ 1.46,  1.47,  1.51,  1.42,  1.48])
lr.predict(X)[setosa_mask][:5]
array([ 1.83762646,  2.1510849 ,  1.52707371,  1.48291658,
 1.52562087])
```

6. Looking at the plots again, we see that the setosa species (upper-left cluster) is largely overestimated by linear regression, and KNN is fairly close to the actual values.

How it works..

KNN regression is very simple to calculate by taking the average of the K closest points to the point being tested. Let's manually predict a single point:

```
example_point = X[0]
```

Now, we need to get the 10 closest points to our `example_point`:

```
from sklearn.metrics import pairwise
distances_to_example = pairwise.pairwise_distances(X)[0]
ten_closest_points = X[np.argsort(distances_to_example)][:10]
ten_closest_y = y[np.argsort(distances_to_example)][:10]
ten_closest_y.mean()
```

```
1.46
```

We can see that this is very close to what was expected.

7

Cross-Validation and Post-Model Workflow

In this chapter, we will cover the following recipes:

- Selecting a model with cross-validation
- K-fold cross-validation
- Balanced cross-validation
- Cross-validation with ShuffleSplit
- Time series cross-validation
- Grid search with scikit-learn
- Randomized search with scikit-learn
- Classification metrics
- Regression metrics
- Clustering metrics
- Using dummy estimators to compare results
- Feature selection
- Feature selection on L1 norms
- Persisting models with joblib or pickle

Introduction

This is perhaps the most important chapter. The fundamental question addressed in this chapter is as follows:

- How do we select a model that predicts well?

This is the purpose of cross-validation, regardless of what the model is. This is slightly different from traditional statistics, which is perhaps more concerned with how we understand a phenomenon better. (Why would I limit my quest for understanding? Well, because there is more and more data, we cannot necessarily look at it all, reflect upon it, and create a theoretical model.)

Machine learning is concerned with prediction and how a machine learning algorithm processes new unseen data and arrives at predictions. Even if it does not seem like traditional statistics, you can use interpretation and domain understanding to create new columns (features) and make even better predictions. You can use traditional statistics to create new columns.

Very early in the book, we started with training/testing splits. Cross-validation is the iteration of many crucial training and testing splits to maximize prediction performance.

This chapter examines the following:

- Cross-validation schemes
- Grid searches—what are the best parameters within an estimator?
- Metrics that compare `y_test` with `y_pred`—the real target set versus the predicted target set

The following line contains the cross-validation scheme `cv = 10` for the scoring mechanism `neg_log_loss`, which is built from the `log_loss` metric:

```
cross_val_score(SVC(), X_train, y_train, cv = 10, scoring='neg_log_loss')
```

Part of the power of scikit-learn is including so much information in a single line. Additionally, we will also see a dummy estimator, have a look at feature selection, and save trained models. These methods are what really make machine learning what it is.

Selecting a model with cross-validation

We saw automatic cross-validation, the `cross_val_score` function, in Chapter 1, *High-Performance Machine Learning – NumPy*. This will be very similar, except we will use the last two columns of the iris dataset as the data. The purpose of this section is to select the best model we can.

Before starting, we will define the best model as the one that scores the highest. If there happens to be a tie, we will choose the model that has the best score with the least volatility.

Getting ready

In this recipe we will do the following:

- Load the last two features (columns) of the iris dataset
- Split the data into training and testing data
- Instantiate two **k-nearest neighbors (KNN)** algorithms, with three and five neighbors
- Score both algorithms
- Select the model that scores the best

Start by loading the dataset:

```
from sklearn import datasets

iris = datasets.load_iris()
X = iris.data[:,2:]
y = iris.target
```

Split the data into training and testing. The samples are stratified, the default throughout the book. Stratified means that the proportions of the target variable are the same in both the training and testing sets (also, `random_state` is set to 7):

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, stratify =
y, random_state = 7)
```


How to do it...

1. First, instantiate two nearest-neighbor algorithms:

```
from sklearn.neighbors import KNeighborsClassifier

kn_3 = KNeighborsClassifier(n_neighbors = 3)
kn_5 = KNeighborsClassifier(n_neighbors = 5)
```

2. Now, score both algorithms using `cross_val_score`. View `kn_3_scores`, a list of scores:

```
from sklearn.model_selection import cross_val_score

kn_3_scores = cross_val_score(kn_3, X_train, y_train, cv=4)
kn_5_scores = cross_val_score(kn_5, X_train, y_train, cv=4)
kn_3_scores

array([ 0.9 , 0.92857143, 0.92592593, 1. ])
```

3. View `kn_5_scores`, the other list of scores:

```
kn_5_scores

array([ 0.96666667, 0.96428571, 0.88888889, 1. ])
```

4. View basic statistics of both lists. View the means:

```
print "Mean of kn_3: ",kn_3_scores.mean()
print "Mean of kn_5: ",kn_5_scores.mean()

Mean of kn_3: 0.938624338624
Mean of kn_5: 0.95496031746
```

5. View the spreads, looking at the standard deviations:

```
print "Std of kn_3: ",kn_3_scores.std()
print "Std of kn_5: ",kn_5_scores.std()

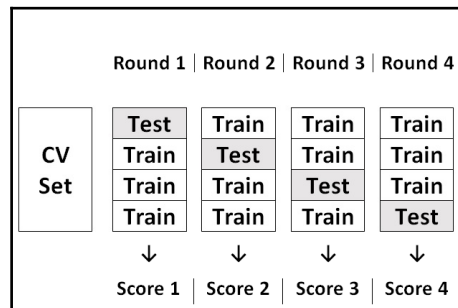
Std of kn_3: 0.037152126551
Std of kn_5: 0.0406755710299
```

Overall, `kn_5`, when the algorithm is set to five neighbors, performs a little better than three neighbors, yet it is less stable (its scores are a bit more all over the place).

6. Let's now do the final step: select the model that scores the highest. We select `kn_5` because it scores the highest. (This model has the highest score under cross-validation. Note that the scores involved are the nearest neighbors default accuracy score: the proportion of correct classifications divided by all of the classifications attempted.)

How it works...

This is an example of 4-fold cross-validation because in the `cross_val_score` function, `cv = 4`. We split the training data, or **CV Set** (`X_train`), into four parts, or folds. We iterate by rotating each fold as the testing set. At first, fold 1 is the testing set while folds 2, 3, and 4 are together the training set. Then fold 2 is the testing set while folds 1, 3, and 4 are the training set. We do this procedure with folds 3 and 4 as well:



Once we split the dataset into folds, we score the algorithm four times:

1. We train one of the nearest neighbors algorithm on folds 2, 3, and 4.
2. Then we predict on fold 1, the test fold.
3. We measure the classification accuracy: compare the test fold with the predicted results on that fold. This is the first of the classification scores on the list.

The process is performed four times. The final output is a list of four scores.

Overall, we did the whole process twice, once for `kn_3` and once for `kn_5`, and produced two lists to select the best model. The module we imported from is called `model_selection` because it is helping us select the best model.

K-fold cross validation

In the quest to find the best model, you can view the indices of cross-validation folds and see what data is in each fold.

Getting ready

Create a toy dataset that is very small:

```
import numpy as np
X = np.array([[1, 2], [3, 4], [5, 6], [7, 8], [1, 2], [3, 4], [5, 6], [7, 8]])
y = np.array([1, 2, 1, 2, 1, 2, 1, 2])
```

How to do it..

1. Import `KFold` and select the number of splits:

```
from sklearn.model_selection import KFold

kf= KFold(n_splits = 4)
```

2. You can iterate through the generator and print out the indices:

```
cc = 1
for train_index, test_index in kf.split(X):
    print "Round : ",cc," : ",
    print "Training indices :", train_index,
    print "Testing indices :", test_index
    cc += 1

Round 1 : Training indices : [2 3 4 5 6 7] Testing indices : [0 1]
Round 2 : Training indices : [0 1 4 5 6 7] Testing indices : [2 3]
Round 3 : Training indices : [0 1 2 3 6 7] Testing indices : [4 5]
Round 4 : Training indices : [0 1 2 3 4 5] Testing indices : [6 7]
```

You can see, for example, how in the first round there are two testing indices, 0 and 1. [0 1] constitutes the first fold. [2 3 4 5 6 7] are folds 2, 3, and 4 put together.

3. You can also view the number of splits:

```
kf.get_n_splits()
```

```
4
```

The number of splits is 4, which we set when we instantiated the `KFold` class.

There's more...

If you want, you can view the data in the folds themselves. Store the generator as a list:

```
indices_list = list(kf.split(X))
```

Now, `indices_list` is a list of tuples. View the information for the fourth fold:

```
indices_list[3] #the list is indexed from 0 to 3
```

```
(array([0, 1, 2, 3, 4, 5], dtype=int64), array([6, 7], dtype=int64))
```

This information matches the information from the preceding printout, except it is in the form of a tuple of two NumPy arrays. View the actual data from the fourth fold. View the training data for the fourth fold:

```
train_indices, test_indices = indices_list[3]
```

```
X[train_indices]
```

```
array([[1, 2],  
       [3, 4],  
       [5, 6],  
       [7, 8],  
       [1, 2],  
       [3, 4]])
```

```
y[train_indices]
```

```
array([1, 2, 1, 2, 1, 2])
```

View the test data:

```
X[test_indices]
```

```
array([[5, 6],  
       [7, 8]])
```

```
y[test_indices]
array([1, 2])
```

Balanced cross-validation

While splitting the different folds in various datasets, you might wonder: couldn't the different sets in each fold of k-fold cross-validation be very different? The distributions could be very different in each fold, and these differences could lead to volatility in the scores.

There is a solution for this, using stratified cross-validation. The subsets of the dataset will look like smaller versions of the whole dataset (at least in the target variable).

Getting ready

Create a toy dataset as follows:

```
import numpy as np
X = np.array([[1, 2], [3, 4], [5, 6], [7, 8], [1, 2], [3, 4], [5, 6], [7, 8]])
y = np.array([1, 1, 1, 1, 2, 2, 2, 2])
```

How to do it...

1. If we perform 4-fold cross-validation on this miniature toy dataset, each of the four testing folds will have only one value for the target. This can be remedied using `StratifiedKFold`:

```
from sklearn.model_selection import StratifiedKFold

skf = StratifiedKFold(n_splits = 4)
```

2. Print out the indices of the folds:

```
cc = 1
for train_index, test_index in skf.split(X,y):
    print "Round",cc,":",
    print "Training indices :", train_index,
    print "Testing indices :", test_index
    cc += 1
```

```

Round 1 : Training indices : [1 2 3 5 6 7] Testing indices : [0 4]
Round 2 : Training indices : [0 2 3 4 6 7] Testing indices : [1 5]
Round 3 : Training indices : [0 1 3 4 5 7] Testing indices : [2 6]
Round 4 : Training indices : [0 1 2 4 5 6] Testing indices : [3 7]

```

Observe that the `split` method of the `skf` class, the stratified k-fold split, has two arguments, `x` and `y`. It tries to distribute the target `y` with the same distribution in each of the fold sets. In this case, every subset has 50% 1 and 50% 2, just like the whole target set `y`.

There's more...

You can use `StratifiedShuffleSplit` to reshuffle the stratified fold. Note that this does not try to make four folds with testing sets that are mutually exclusive:

```

from sklearn.model_selection import StratifiedShuffleSplit

sss = StratifiedShuffleSplit(n_splits = 5, test_size=0.25)

cc = 1
for train_index, test_index in sss.split(X,y):
    print "Round",cc,":",
    print "Training indices :", train_index,
    print "Testing indices :", test_index
    cc += 1

Round 1 : Training indices : [1 6 5 7 0 2] Testing indices : [4 3]
Round 2 : Training indices : [3 2 6 7 5 0] Testing indices : [1 4]
Round 3 : Training indices : [2 1 4 7 0 6] Testing indices : [3 5]
Round 4 : Training indices : [4 2 7 6 0 1] Testing indices : [5 3]
Round 5 : Training indices : [1 2 0 5 4 7] Testing indices : [6 3]
Round 6 : Training indices : [0 6 5 1 7 3] Testing indices : [2 4]
Round 7 : Training indices : [1 7 3 6 2 5] Testing indices : [0 4]

```

The splits are not splits of the dataset but iterations of a random procedure, each one with a training set size of 75% of the whole dataset and a testing set size of 25%. All of the iterations are stratified.

Cross-validation with ShuffleSplit

The ShuffleSplit is one of the simplest cross-validation techniques. Using this cross-validation technique will simply take a sample of the data for the number of iterations specified.

Getting ready

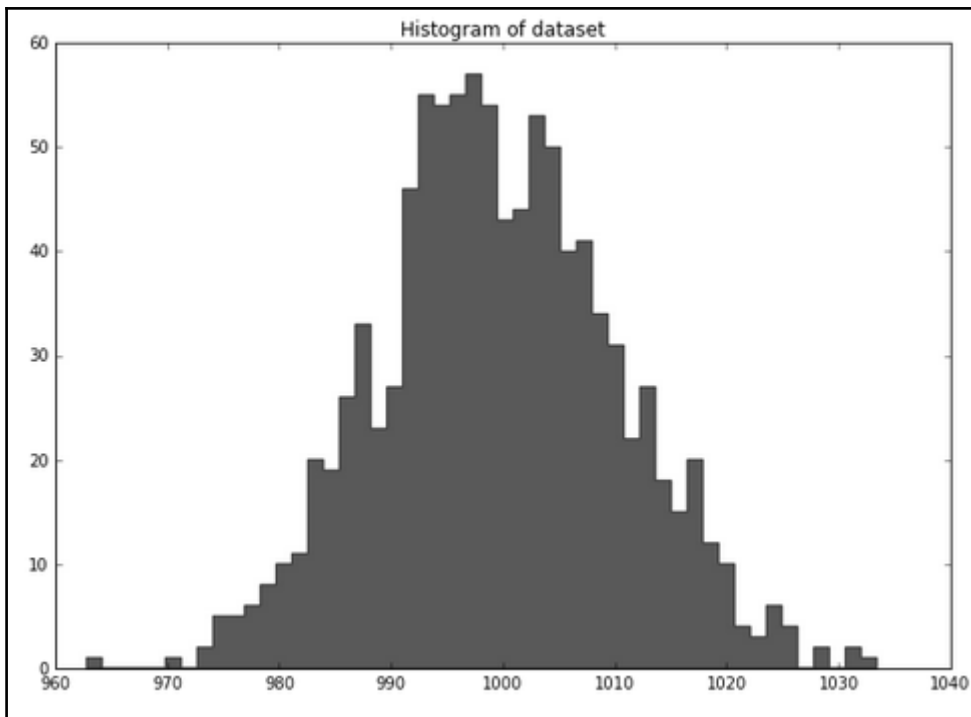
The ShuffleSplit is a simple validation technique. We'll specify the total elements in the dataset, and it will take care of the rest. We'll walk through an example of estimating the mean of a univariate dataset. This is similar to resampling, but it'll illustrate why we want to use cross-validation while showing cross-validation.

How to do it...

1. First, we need to create the dataset. We'll use NumPy to create a dataset in which we know the underlying mean. We'll sample half of the dataset to estimate the mean and see how close it is to the underlying mean. Generate a normally distributed random sample with a mean of 1,000 and a scale (standard deviation) of 10:

```
%matplotlib inline

import numpy as np
true_mean = 1000
true_std = 10
N = 1000
dataset = np.random.normal(loc= true_mean, scale = true_std,
size=N)
import matplotlib.pyplot as plt
f, ax = plt.subplots(figsize=(10, 7))
ax.hist(dataset, color='k', alpha=.65,
histtype='stepfilled',bins=50)
ax.set_title("Histogram of dataset")
```



2. Estimate the mean of half of the dataset:

```
holdout_set = dataset[:500]
fitting_set = dataset[500:]
estimate = fitting_set[:N/2].mean()
estimate
```

```
999.69789261486721
```

3. You can also get the mean of the whole dataset:

```
data_mean = dataset.mean()
data_mean
```

```
999.55177343767843
```

4. It is not 1,000 because random points were selected to create the dataset. To observe the behavior of `ShuffleSplit`, write the following and make a plot:

```
from sklearn.model_selection import ShuffleSplit
shuffle_split = ShuffleSplit(n_splits=100, test_size=.5,
                             random_state=0)
```

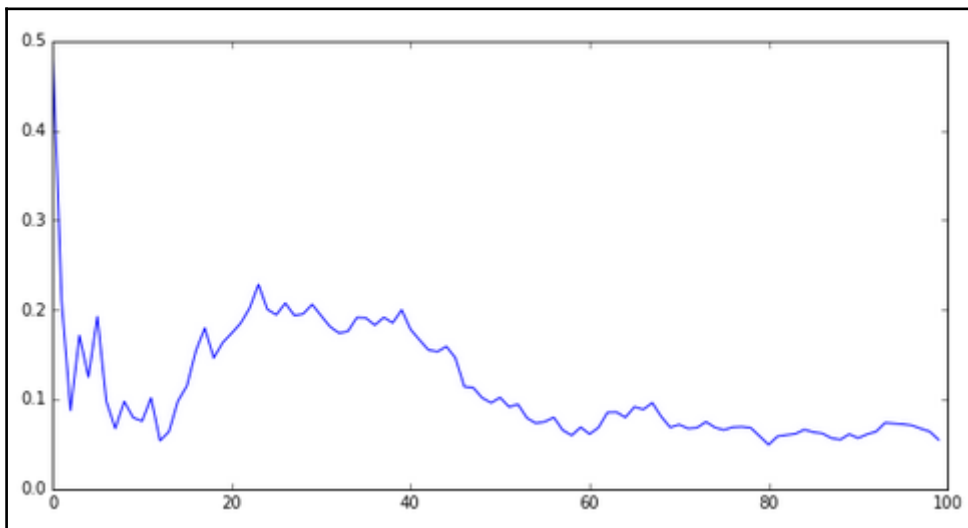


```

mean_p = []
estimate_closeness = []
for train_index, not_used_index in
    shuffle_split(fitting_set):
        mean_p.append(fitting_set[train_index].mean())
        shuf_estimate = np.mean(mean_p)
        estimate_closeness.append(np.abs(shuf_estimate -
            dataset.mean()))

plt.figure(figsize=(10,5))
plt.plot(estimate_closeness)

```



The estimated mean keeps getting closer to the data's mean of 999.55177343767843 and then plateaus at being 0.1 away from the data's mean. It is a bit closer than the estimate of the mean, with half the dataset, to the mean of the data.

Time series cross-validation

scikit-learn can perform cross-validation for time series data such as stock market data. We will do so with a time series split, as we would like the model to predict the future, not have an information data leak from the future.

Getting ready

We will create the indices for a time series split. Start by creating a small toy dataset:

```
from sklearn.model_selection import TimeSeriesSplit
import numpy as np
X = np.array([[1, 2], [3, 4], [1, 2], [3, 4], [1, 2], [3, 4], [1, 2], [3, 4]])
y = np.array([1, 2, 3, 4, 1, 2, 3, 4])
```

How to do it...

1. Now create a time series split object:

```
tscv = TimeSeriesSplit(n_splits=7)
```

2. Iterate through it:

```
for train_index, test_index in tscv.split(X):

    X_train, X_test = X[train_index], X[test_index]
    y_train, y_test = y[train_index], y[test_index]

    print "Training indices:", train_index, "Testing indices:",
    test_index

Training indices: [0] Testing indices: [1]
Training indices: [0 1] Testing indices: [2]
Training indices: [0 1 2] Testing indices: [3]
Training indices: [0 1 2 3] Testing indices: [4]
Training indices: [0 1 2 3 4] Testing indices: [5]
Training indices: [0 1 2 3 4 5] Testing indices: [6]
Training indices: [0 1 2 3 4 5 6] Testing indices: [7]
```

3. You can also save the indices by creating a list of tuples from the generator:

```
tscv_list = list(tscv.split(X))
```

There's more...

You can create rolling windows with NumPy or pandas as well. The main requirement of time series cross-validation is that the test set appears after the training set in time; otherwise, you would be predicting the past from the future.

Time series cross-validation is interesting because depending on the dataset, the influence of time varies. Sometimes, you do not have to put data rows in time-sequential order, yet you can never assume you know the future in the past.

Grid search with scikit-learn

At the beginning of the model selection and cross-validation chapter we tried to select the best nearest-neighbor model for the two last features of the iris dataset. We will refocus on that now with `GridSearchCV` in scikit-learn.

Getting ready

First, load the last two features of the iris dataset. Split the data into training and testing sets:

```
from sklearn import datasets

iris = datasets.load_iris()
X = iris.data[:,2:]
y = iris.target

from sklearn.model_selection import train_test_split,
cross_val_score

X_train, X_test, y_train, y_test = train_test_split(X, y, stratify
= y, random_state = 7)
```

How to do it...

1. Instantiate a nearest neighbors classifier:

```
from sklearn.neighbors import KNeighborsClassifier

knn_clf = KNeighborsClassifier()
```

2. Prepare a parameter grid, which is necessary for a grid search. A parameter grid is a dictionary with the parameter setting you would like to try:

```
param_grid = {'n_neighbors': list(range(3,9,1))}
```

3. Instantiate a grid search passing the following as arguments:

- The estimator
- The parameter grid
- A type of cross-validation, `cv=10`

```
from sklearn.model_selection import GridSearchCV
gs = GridSearchCV(knn_clf, param_grid, cv=10)
```

4. Fit the grid search estimator:

```
gs.fit(X_train, y_train)
```

5. View the results:

```
gs.best_params_

{'n_neighbors': 3}

gs.cv_results_['mean_test_score']

zip(gs.cv_results_['params'], gs.cv_results_['mean_test_score'])

[({'n_neighbors': 3}, 0.9553571428571429),
 ({'n_neighbors': 4}, 0.9375),
 ({'n_neighbors': 5}, 0.9553571428571429),
 ({'n_neighbors': 6}, 0.9553571428571429),
 ({'n_neighbors': 7}, 0.9553571428571429),
 ({'n_neighbors': 8}, 0.9553571428571429)]
```

How it works...

In the first chapter, we tried the brute force method, that is, scanning for the best score with Python:

```
all_scores = []
for n_neighbors in range(3,9,1):
    knn_clf = KNeighborsClassifier(n_neighbors = n_neighbors)
    all_scores.append((n_neighbors, cross_val_score(knn_clf, X_train,
y_train, cv=10).mean()))
    sorted(all_scores, key = lambda x:x[1], reverse = True)

[(3, 0.9566666666666667),
 (5, 0.9566666666666667),
 (6, 0.9566666666666667),
 (7, 0.9566666666666667),
```

```
(8, 0.9566666666666667),  
(4, 0.94000000000000006)]
```

The problem with this approach is that it is more time consuming and error prone, especially if there are more parameters involved or additional transformations, such as those involved in using pipelines.

Note that the grid search and brute force approaches both scan all of the possible values of the parameters.

Randomized search with scikit-learn

From a practical standpoint, `RandomizedSearchCV` is more important than a regular grid search. This is because with a medium amount of data, or with a model involving a few parameters, it is too computationally expensive to try every parameter combination involved in a complete grid search.

Computational resources are probably better spent stratifying sampling very well, or improving randomization procedures.

Getting ready

As before, load the last two features of the iris dataset. Split the data into training and testing sets:

```
from sklearn import datasets  
  
iris = datasets.load_iris()  
X = iris.data[:,2:]  
y = iris.target  
  
from sklearn.model_selection import train_test_split  
  
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify =  
y, random_state = 7)
```

How to do it...

1. Instantiate a nearest neighbors classifier:

```
from sklearn.neighbors import KNeighborsClassifier

knn_clf = KNeighborsClassifier()
```

2. Prepare a parameter distribution, which is necessary for a randomized grid search. A parameter distribution is a dictionary with the parameter setting you would like to try randomly:

```
param_dist = {'n_neighbors': list(range(3, 9, 1))}
```

3. Instantiate a randomized grid search passing the following as arguments:

- The estimator
- The parameter distribution
- A type of cross-validation, `cv=10`
- The number of times to run the procedure, `n_iter`

```
from sklearn.model_selection import RandomizedSearchCV
rs = RandomizedSearchCV(knn_clf, param_dist, cv=10, n_iter=6)
```

4. Fit the randomized grid search estimator:

```
rs.fit(X_train, y_train)
```

5. View the results:

```
rs.best_params_

{'n_neighbors': 3}

zip(rs.cv_results_['params'], rs.cv_results_['mean_test_score'])

[({'n_neighbors': 3}, 0.9553571428571429),
 ({'n_neighbors': 4}, 0.9375),
 ({'n_neighbors': 5}, 0.9553571428571429),
 ({'n_neighbors': 6}, 0.9553571428571429),
 ({'n_neighbors': 7}, 0.9553571428571429),
 ({'n_neighbors': 8}, 0.9553571428571429)]
```

6. In this case, we actually ran a grid search through all six of the parameters. You could have scanned a larger parameter space, however:

```
param_dist = {'n_neighbors': list(range(3,50,1))}
rs = RandomizedSearchCV(knn_clf,param_dist,cv=10,n_iter=15)
rs.fit(X_train,y_train)

rs.best_params_

{'n_neighbors': 16}
```

7. Try timing this procedure with IPython:

```
%timeit rs.fit(X_train,y_train)

1 loop, best of 3: 1.06 s per loop
```

8. Time the grid search procedure:

```
from sklearn.model_selection import GridSearchCV
param_grid = {'n_neighbors': list(range(3,50,1))}
gs = GridSearchCV(knn_clf,param_grid,cv=10)

%timeit gs.fit(X_train,y_train)

1 loop, best of 3: 3.24 s per loop
```

9. Look at the grid search's best parameters:

```
gs.best_params_

{'n_neighbors': 3}
```

10. It turns out that 3-nearest neighbors scores the same as 16-nearest neighbors:

```
zip(gs.cv_results_['params'],gs.cv_results_['mean_test_score'])

[({'n_neighbors': 3}, 0.9553571428571429),
 ({'n_neighbors': 4}, 0.9375),
 ...
 ({'n_neighbors': 14}, 0.9553571428571429),
 ({'n_neighbors': 15}, 0.9553571428571429),
 ({'n_neighbors': 16}, 0.9553571428571429),
 ({'n_neighbors': 17}, 0.9464285714285714),
 ...]
```

Thus, we got the same score in one-third of the time.



Whether to use randomized search or not is a decision you have to make on a case-by-case basis. You should use a randomized search to try to get a feel for an algorithm. It is possible that it performs poorly no matter what the parameters are, so then you can move on to a different algorithm. If the algorithm performs very well, you can use a complete grid search to find the best parameters.

Additionally, instead of focusing on exhaustive searches, you could bag, stack, or mix a set of reasonably good algorithms.

Classification metrics

Earlier in the chapter, we explored choosing the best of a few nearest neighbors instances based on the number of neighbors, `n_neighbors`, parameter. This is the main parameter in nearest neighbors classification: classify a point based on the label of KNN. So, for 3-nearest neighbors, classify a point based on the label of the three nearest points. Take a majority vote of the three nearest points.

The classification metric in this case was the internal metric `accuracy_score`, which is defined as the number of classifications that were correct divided by the total number of classifications. There are alternate metrics, and we will explore them here.

Getting ready

1. To start, load the Pima diabetes dataset from the UCI repository:

```
import pandas as pd

data_web_address =
"https://archive.ics.uci.edu/ml/machine-learning-databases/pima-ind
ians-diabetes/pima-indians-diabetes.data"

column_names = ['pregnancy_x',
'plasma_con',
'blood_pressure',
'skin_mm',
'insulin',
'bmi',
'pedigree_func',
```



```
'age',
'target']

feature_names = column_names[:-1]
all_data = pd.read_csv(data_web_address , names=column_names)
```

2. Split the data into training and testing sets:

```
import numpy as np
import pandas as pd

X = all_data[feature_names]
y = all_data['target']

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=7, stratify=y)
```

3. To review the previous section, run a randomized search using the KNN algorithm:

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import RandomizedSearchCV

knn_clf = KNeighborsClassifier()

param_dist = {'n_neighbors': list(range(3,20,1))}

rs = RandomizedSearchCV(knn_clf,param_dist,cv=10,n_iter=17)
rs.fit(X_train, y_train)
```

4. Then display the best accuracy score:

```
rs.best_score_

0.75407166123778502
```

5. Additionally, look at the confusion matrix on the test set:

```
y_pred = rs.predict(X_test)

from sklearn.metrics import confusion_matrix

confusion_matrix(y_test, y_pred)

array([[84, 16],
       [27, 27]])
```

The confusion matrix gives more specific information about how the model performed. There were 27 times when the model predicted someone did not have diabetes even though they did. This is a more serious mistake than the 16 people thought to have diabetes that really did not.

In this situation, we want to maximize sensitivity or recall. While examining linear models, we looked at the definition of recall, or sensitivity:

$$\text{Sensitivity} = \frac{\text{People correctly labelled having diabetes}}{\text{All people who have diabetes}}$$

Thus, the sensitivity score in this case is $27 / (27 + 27) = 0.5$. With scikit-learn, we can conveniently compute this as follows.

How to do it...

1. Import from the metrics module `recall_score`. Measure the sensitivity of the set using `y_test` and `y_pred`:

```
from sklearn.metrics import recall_score

recall_score(y_test, y_pred)

0.5
```

We recovered the recall score we computed by hand beforehand. In the randomized search, we could have used the `recall_score` to find the nearest neighbor instance with the highest recall.

2. Import `make_scorer` and use the function with two arguments, `recall_score` and `greater_is_better`:

```
from sklearn.metrics import make_scorer

recall_scorer = make_scorer(recall_score, greater_is_better=True)
```

3. Now perform a randomized grid search:

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import RandomizedSearchCV

knn_clf = KNeighborsClassifier()

param_dist = {'n_neighbors': list(range(3, 20, 1))}

rs =
RandomizedSearchCV(knn_clf, param_dist, cv=10, n_iter=17, scoring=recall_scorer)

rs.fit(X_train, y_train)
```

4. Now look at the highest score:

```
rs.best_score_

0.5649632669176643
```

5. Look at the recall score:

```
y_pred = rs.predict(X_test)
recall_score(y_test, y_pred)

0.5
```

6. It is the same as before. In the randomized search you could have tried the `roc_auc_score`, the ROC area under the curve:

```
from sklearn.metrics import roc_auc_score

rs =
RandomizedSearchCV(knn_clf, param_dist, cv=10, n_iter=17, scoring=make_scorer(roc_auc_score, greater_is_better=True))

rs.fit(X_train, y_train)

rs.best_score_

0.7100264217324479
```

There's more...

You could design your own scorer for classification. Suppose that you are an insurance company and that you have associated costs for each cell in the confusion matrix. The relative costs are as follows:

Person correctly labelled as not having condition: \$1	Person incorrectly labelled having the condition. \$2 for additional testing
Person incorrectly labelled as not having condition: \$100 : costs in eventually finding and treating condition with complications	Person correctly labelled as having condition: \$20 for treatment

The cost for the confusion matrix we were looking at can be computed as follows:

```
costs_array = confusion_matrix(y_test, y_pred) * np.array([[1,2],
                                                           [100,20]])
costs_array

array([[ 84,   32],
       [2700,  540]])
```

Now add up the total cost:

```
costs_array.sum()

3356
```

Now place it in a scorer and run the grid search. The argument within the scorer `greater_is_better` is set to `False`, because costs should be as low as possible:

```
def costs_total(y_test, y_pred):

    return (confusion_matrix(y_test, y_pred) * np.array([[1,2],
                                                           [100,20]])) .sum()

costs_scorer = make_scorer(costs_total, greater_is_better=False)
```

```
rs =  
RandomizedSearchCV(knn_clf,param_dist,cv=10,n_iter=17,scoring=costs_scorer)  
  
rs.fit(X_train, y_train)  
  
rs.best_score_  
  
-1217.5879478827362
```

The score is negative because when the `greater_is_better` argument in the `make_scorer` function is false, the score is multiplied by `-1`. The grid search attempts to maximize this score, thereby minimizing the absolute value of the score.

The cost on the test set is as follows:

```
costs_total(y_test,rs.predict(X_test))  
  
3356
```

While looking at this number, do not forget to look at the number of individuals involved in the test set, which is 154. The average cost per person is about \$21.8.

Regression metrics

Cross-validation with a regression metric is straightforward with scikit-learn. Either import a score function from `sklearn.metrics` and place it within a `make_scorer` function, or you could create a custom scorer for a particular data science problem.

Getting ready

Load a dataset that utilizes a regression metric. We will load the Boston housing dataset and split it into training and test sets:

```
from sklearn.datasets import load_boston  
boston = load_boston()  
  
X = boston.data  
y = boston.target  
  
from sklearn.model_selection import train_test_split, cross_val_score  
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,  
random_state=7)
```

We do not know much about the dataset. We can try a quick grid search using a high variance algorithm:

```
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import RandomizedSearchCV

knn_reg = KNeighborsRegressor()
param_dist = {'n_neighbors': list(range(3, 20, 1))}
rs = RandomizedSearchCV(knn_reg, param_dist, cv=10, n_iter=17)
rs.fit(X_train, y_train)
rs.best_score_

0.46455839325055914
```

Try a different model, this time a linear model:

```
from sklearn.linear_model import Ridge
cross_val_score(Ridge(), X_train, y_train, cv=10).mean()

0.7439511908709866
```

Both regressors, by default, measure `r2_score`, R-squared, so the linear model is far better. Try a different complex model, an ensemble of trees:

```
from sklearn.ensemble import GradientBoostingRegressor,
RandomForestRegressor
cross_val_score(GradientBoostingRegressor(max_depth=7), X_train, y_train, cv=10).mean()

0.83082671732165492
```

The ensemble performs even better. You can try a random forest as well:

```
cross_val_score(RandomForestRegressor(), X_train, y_train, cv=10).mean()

0.82474734196711685
```

Now we could focus on making gradient boosting better with the current score mechanism by maximizing the internal R-squared gradient boosting scorer. Try one or two randomized searches. This is a second one:

```
param_dist = {'n_estimators': [4000], 'learning_rate': [0.01],
              'max_depth': [1, 2, 3, 5, 7]}
rs_inst_a = RandomizedSearchCV(GradientBoostingRegressor(), param_dist,
n_iter = 5, n_jobs=-1)
rs_inst_a.fit(X_train, y_train)
```

Optimizing for R-squared returned the following:

```
rs_inst_a.best_params_  
  
{'learning_rate': 0.01, 'max_depth': 3, 'n_estimators': 4000}  
  
rs_inst_a.best_score_  
  
0.88548410382780185
```

The trees in the gradient boost have a depth of three.

How to do it...

Now we will do the following:

1. Make a scoring function.
2. Make a scikit-scorer with that function.
3. Run a grid search to find the best gradient boost parameters to minimize the error function.

Let's start:

1. Make the mean percentage error scoring function with the Numba **just-in-time (JIT)** compiler. The original NumPy function looks like this:

```
def mape_score(y_test, y_pred):  
    return (np.abs(y_test - y_pred)/y_test).mean()
```

2. Let's rewrite the function using the Numba JIT compiler to make things a bit faster. You can write C-like code, indexing arrays by location using Numba:

```
from numba import autojit  
  
@autojit  
def mape_score(y_test, y_pred):  
    sum_total = 0  
    y_vec_length = len(y_test)  
    for index in range(y_vec_length):  
        sum_total += (1 - (y_pred[index]/y_test[index]))  
  
    return sum_total/y_vec_length
```

3. Now make a scorer. The lower the score the better, unlike R-squared, in which higher is better:

```
from sklearn.metrics import make_scorer
mape_scorer = make_scorer(mape_score, greater_is_better=False)
```

4. Now run a grid search:

```
param_dist = {'n_estimators': [4000], 'learning_rate': [0.01],
              'max_depth': [1, 2, 3, 4, 5]}
rs_inst_b = RandomizedSearchCV(GradientBoostingRegressor(),
                               param_dist, n_iter = 3, n_jobs=-1, scoring = mape_scorer)
rs_inst_b.fit(X_train, y_train)
rs_inst_b.best_score_

0.021086502313661441

rs_inst_b.best_params_

{'learning_rate': 0.01, 'max_depth': 1, 'n_estimators': 4000}
```

Using this metric, the best score corresponds to a gradient boost with trees of depth one.

Clustering metrics

Measuring the performance of a clustering algorithm is a little trickier than classification or regression, because clustering is unsupervised machine learning. Thankfully, scikit-learn comes equipped to help us with this as well in a very straightforward manner.

Getting ready

To measure clustering performance, start by loading the iris dataset. We will relabel the iris flowers as two types: type 0 is whenever the target is 0 and type 1 is when the target is 1 or 2:

```
from sklearn.datasets import load_iris
import numpy as np

iris = load_iris()
X = iris.data
y = np.where(iris.target == 0, 0, 1)
```


How to do it...

1. Instantiate a k-means algorithm and train it. Since the algorithm is a clustering one, do not use the target in the training:

```
from sklearn.cluster import KMeans

kmeans = KMeans(n_clusters=2, random_state=0)
kmeans.fit(X)
```

2. Now import everything necessary to score k-means through cross-validation. We will use the `adjusted_rand_score` clustering performance metric:

```
from sklearn.metrics.cluster import adjusted_rand_score
from sklearn.metrics import make_scorer
from sklearn.model_selection import cross_val_score

cross_val_score(kmeans, X, y, cv=10, scoring=make_scorer(adjusted_rand_score)).mean()

0.8733695652173914
```

Scoring a clustering algorithm is very similar to scoring a classification algorithm.

Using dummy estimators to compare results

This recipe is about creating fake estimators; this isn't the pretty or exciting stuff, but it is worthwhile having a reference point for the model you'll eventually build.

Getting ready

In this recipe, we'll perform the following tasks:

1. Create some random data.
2. Fit the various dummy estimators.

We'll perform these two steps for regression data and classification data.

How to do it...

1. First, we'll create the random data:

```
from sklearn.datasets import make_regression, make_classification

X, y = make_regression()
from sklearn import dummy
dumdum = dummy.DummyRegressor()
dumdum.fit(X, y)

DummyRegressor(constant=None, quantile=None, strategy='mean')
```

2. By default, the estimator will predict by just taking the mean of the values and outputting it multiple times::

```
dumdum.predict(X) [:5]

>array([-25.0450033, -25.0450033, -25.0450033, -25.0450033,
       -25.0450033])
```

There are other two other strategies we can try. We can predict a supplied constant (refer to `constant=None` in the first command block in this recipe). We can also predict the median value. Supplying a constant will only be considered if strategy is constant.

3. Let's have a look:

```
predictors = [("mean", None),
              ("median", None),
              ("constant", 10)]
for strategy, constant in predictors:
    dumdum = dummy.DummyRegressor(strategy=strategy,
                                   constant=constant)
    dumdum.fit(X, y)
    print "strategy: {}".format(strategy), ", ".join(map(str,
dumdum.predict(X) [:5]))

strategy: mean
-25.0450032962, -25.0450032962, -25.0450032962, -25.0450032962, -25.045
0032962
strategy: median
-37.734448002, -37.734448002, -37.734448002, -37.734448002, -37.7344480
02
strategy: constant 10.0, 10.0, 10.0, 10.0, 10.0
```

4. We actually have four options for classifiers. These strategies are similar to the continuous case, it's just slanted toward classification problems:

```

predictors = [("constant", 0), ("stratified", None), ("uniform",
None), ("most_frequent", None)]
#We'll also need to create some classification data:
X, y = make_classification()
for strategy, constant in predictors:
    dumdummy = dummy.DummyClassifier(strategy=strategy,
    constant=constant)
    dumdummy.fit(X, y)
    print "strategy: {}".format(strategy),
    ", ".join(map(str, dumdummy.predict(X)[:5]))

strategy: constant 0,0,0,0,0
strategy: stratified 1,0,1,1,1
strategy: uniform 1,0,1,0,1
strategy: most_frequent 0,0,0,0,0

```

How it works...

It's always good to test your models against the simplest models, and that's exactly what the dummy estimators give you. For example, imagine a fraud model. In this model, only 5% of the dataset is fraudulent. Therefore, we can probably fit a pretty good model just by never guessing that the data is fraudulent.

We can create this model by using the stratified strategy using the following command. We can also get a good example of why class imbalance causes problems:

```

X, y = make_classification(20000, weights=[.95, .05])
dumdummy = dummy.DummyClassifier(strategy='most_frequent')
dumdummy.fit(X, y)

DummyClassifier(constant=None, random_state=None, strategy='most_frequent')

from sklearn.metrics import accuracy_score
print accuracy_score(y, dumdummy.predict(X))

0.94615

```

We were actually correct very often, but that's not the point. The point is that this is our baseline. If we cannot create a model for fraud that is more accurate than this, then it isn't worth our time.

Feature selection

This recipe, along with the two following it, will be centered around automatic feature selection. I like to think of this as the feature analog of parameter tuning. In the same way that we cross-validate to find an appropriately general parameter, we can find an appropriately general subset of features. This will involve several different methods. The simplest idea is univariate selection. The other methods involve working with a combination of features.

An added benefit of feature selection is that it can ease the burden on the data collection. Imagine that you have built a model on a very small subset of the data. If all goes well, you might want to scale up to predict the model on the entire subset of data. If this is the case, you can ease the engineering effort of data collection at that scale.

Getting ready

With univariate feature selection, scoring functions will come to the forefront again. This time, they will define the comparable measure by which we can eliminate features.

In this recipe, we'll fit a regression model with around 10,000 features, but only 1,000 points. We'll walk through the various univariate feature selection methods:

```
from sklearn import datasets
X, y = datasets.make_regression(1000, 10000)
```

Now that we have the data, we will compare the features that are included with the various methods. This is actually a very common situation when you're dealing with text analysis or some areas of bioinformatics.

How to do it...

1. First, we need to import the `feature_selection` module:

```
from sklearn import feature_selection
f, p = feature_selection.f_regression(X, y)
```

- Here, f is the f score associated with each linear model fit with just one of the features. We can then compare these features and based on this comparison, we can cull features. p is the p value associated with the f value. In statistics, the p value is the probability of a value more extreme than the current value of the test statistic. Here, the f value is the test statistic:

```
f[:5]

array([ 1.23494617,  0.70831694,  0.09219176,  0.14583189,
        0.78776466])

p[:5]

array([ 0.26671492,  0.40020473,  0.76147235,  0.7026321 ,
        0.37499074])
```

- As we can see, many of the p values are quite large. We want the p values to be quite small. So, we can grab NumPy out of our toolbox and choose all the p values less than .05. These will be the features we'll use for our analysis:

```
import numpy as np
idx = np.arange(0, X.shape[1])
features_to_keep = idx[p < .05]
len(features_to_keep)

496
```

As you can see, we're actually keeping a relatively large number of features. Depending on the context of the model, we can tighten this p value. This will lessen the number of features kept.

Another option is using the `VarianceThreshold` object. We've learned a bit about it, but it's important to understand that our ability to fit models is largely based on the variance created by features. If there is no variance, then our features cannot describe the variation in the dependent variable. A nice feature of this, as per the documentation, is that because it does not use the outcome variable, it can be used for unsupervised cases.

- We will need to set the threshold for which we eliminate features. In order to do that, we just take the median of the feature variances and supply that:

```
var_threshold =
feature_selection.VarianceThreshold(np.median(np.var(X, axis=1)))
var_threshold.fit_transform(X).shape
```

```
(1000L, 4888L)
```

As we can see, we have eliminated roughly half the features, more or less what we would expect.

How it works...

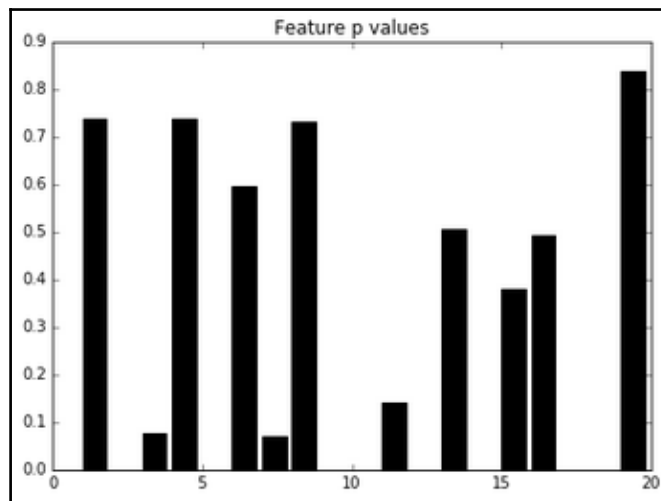
In general, all these methods work by fitting a basic model with a single feature. Depending on whether we have a classification problem or a regression problem, we can use the appropriate scoring function.

Let's look at a smaller problem and visualize how feature selection will eliminate certain features. We'll use the same scoring function from the first example, but just 20 features:

```
X, y = datasets.make_regression(10000, 20)
f, p = feature_selection.f_regression(X, y)
```

Now let's plot the p values of the features. We can see which features will be eliminated and which will be kept:

```
%matplotlib inline
from matplotlib import pyplot as plt
f, ax = plt.subplots(figsize=(7, 5))
ax.bar(np.arange(20), p, color='k')
ax.set_title("Feature p values")
```



As we can see, many of the features won't be kept, but several will be.

Feature selection on L1 norms

We're going to work with some ideas that are similar to those we saw in the recipe on LASSO regression. In that recipe, we looked at the number of features that had zero coefficients. Now we're going to take this a step further and use the sparseness associated with L1 norms to pre-process the features.

Getting ready

We'll use the diabetes dataset to fit a regression. First, we'll fit a basic linear regression model with a ShuffleSplit cross-validation. After we do that, we'll use LASSO regression to find the coefficients that are zero when using an L1 penalty. This hopefully will help us to avoid overfitting (when the model is too specific to the data it was trained on). To put this another way, the model, if it overfits, does not generalize well to outside data.

We're going to perform the following steps:

1. Load the dataset.
2. Fit a basic linear regression model.
3. Use feature selection to remove uninformative features.
4. Refit the linear regression and check to see how well it fits compared with the fully featured model.

How to do it...

1. First, let's get the dataset:

```
import sklearn.datasets as ds
diabetes = ds.load_diabetes()

X = diabetes.data
y = diabetes.target
```

2. Let's create the LinearRegression object:

```
from sklearn.linear_model import LinearRegression
lr = LinearRegression()
```

3. Let's also import from the metrics module the `mean_squared_error` function and `make_scorer` wrapper. From the `model_selection` module, import the `ShuffleSplit` cross-validation scheme and the `cross_val_score` cross-validation scorer. Go ahead and score the function with the `mean_squared_error` metric:

```
from sklearn.metrics import make_scorer, mean_squared_error
from sklearn.model_selection import cross_val_score, ShuffleSplit

shuff = ShuffleSplit(n_splits=10, test_size=0.25, random_state=0)
score_before =
cross_val_score(lr, X, y, cv=shuff, scoring=make_scorer(mean_squared_error, greater_is_better=False)).mean()

score_before

-3053.393446308266
```

4. So now that we have the regular fit, let's check it after eliminating any features with a zero for the coefficient. Let's fit the LASSO regression:

```
from sklearn.linear_model import LassoCV

lasso_cv = LassoCV()
lasso_cv.fit(X, y)
lasso_cv.coef_

array([-0. , -226.2375274 , 526.85738059, 314.44026013,
       -196.92164002,  1.48742026, -151.78054083, 106.52846989,
        530.58541123,  64.50588257])
```

5. We'll remove the first feature. I'll use a NumPy array to represent the columns that are to be included in the model:

```
import numpy as np
columns = np.arange(X.shape[1])[lasso_cv.coef_ != 0]
columns
```


6. Okay, so now we'll fit the model with the specific features (see the columns in the following code block):

```
score_afterwards = cross_val_score(lr,X[:,columns],y,cv=shuff,
scoring=make_scorer(mean_squared_error,greater_is_better=False)).mean()
score_afterwards

-3033.5012859289677
```

The score afterwards is not much better than the score before, even though we eliminated an uninformative feature. We will see an additional example in the *There's more...* section.

There's more...

1. First, we're going to create a regression dataset with many uninformative features:

```
X, y = ds.make_regression(noise=5)
```

2. Create a `ShuffleSplit` instance with 10 iterations, `n_splits=10`. Measure the cross-validation score of plain linear regression:

```
shuff = ShuffleSplit(n_splits=10, test_size=0.25, random_state=0)

score_before = cross_val_score(lr,X,y,cv=shuff,
scoring=make_scorer(mean_squared_error,greater_is_better=False)).mean()
```

3. Instantiate `LassoCV` to eliminate uninformative columns:

```
lasso_cv = LassoCV()
lasso_cv.fit(X,y)
```

4. Eliminate uninformative columns. Look at the final scores:

```
columns = np.arange(X.shape[1])[lasso_cv.coef_ != 0]
score_afterwards = cross_val_score(lr,X[:,columns],y,cv=shuff,
scoring=make_scorer(mean_squared_error,greater_is_better=False)).mean()
print "Score before:",score_before
print "Score after: ",score_afterwards

Score before: -8891.35368845
Score after: -22.3488585347
```

The fit is a lot better at the end after we removed uninformative features.

Persisting models with joblib or pickle

In this recipe, we're going to show how you can keep your model around for later use. For example, you might want to actually use a model to predict an outcome and automatically make a decision.

Getting ready

Create a dataset and train a classifier:

```
from sklearn.datasets import make_classification
from sklearn.tree import DecisionTreeClassifier

X, y = make_classification()
dt = DecisionTreeClassifier()
dt.fit(X, y)
```

How to do it...

1. Save the training work the classifier has done with joblib:

```
from sklearn.externals import joblib
joblib.dump(dt, "dtree.clf")

['dtree.clf']
```

Opening the saved model

2. Load the model with joblib. Make a prediction with a set of inputs:

```
from sklearn.externals import joblib
pulled_model = joblib.load("dtree.clf")
y_pred = pulled_model.predict(X)
```

We did not have to train the model again, and have saved a lot of training time. We simply reloaded it with joblib and made a prediction.

There's more...

You can also use the `cPickle` module in Python 2.x or the `pickle` module in Python 3.x. Personally, I use this module for several types of Python classes and objects:

1. Begin by importing `pickle`:

```
import cPickle as pickle #Python 2.x
# import pickle          # Python 3.x
```

2. Use the `dump()` module method. It has three arguments: the data being saved, the file it is being saved to, and the pickle protocol. The following saves the trained tree to the `dtree.save` file:

```
f = open("dtree.save", 'wb')
pickle.dump(dt, f, protocol = pickle.HIGHEST_PROTOCOL)
f.close()
```

3. Open `dtree.save` as follows:

```
f = open("dtree.save", 'rb')
return_tree = pickle.load(f)
f.close()
```

4. View the tree:

```
return_tree

DecisionTreeClassifier(class_weight=None, criterion='gini',
max_depth=None,
                        max_features=None, max_leaf_nodes=None,
                        min_impurity_split=1e-07, min_samples_leaf=1,
                        min_samples_split=2, min_weight_fraction_leaf=0.0,
                        presort=False, random_state=None, splitter='best')
```

8

Support Vector Machines

In this chapter, we will cover these recipes:

- Classifying data with a linear SVM
- Optimizing an SVM
- Multiclass classification with SVM
- Support vector regression

Introduction

In this chapter, we will start by using a **support vector machine (SVM)** with a linear kernel to get a rough idea of how SVMs work. They create a hyperplane, or linear surface in several dimensions, which best separates the data.

In two dimensions, this is easy to see: the hyperplane is a line that separates the data. We will see the array of coefficients and intercept of the SVM. Together they uniquely describe a scikit-learn linear SVC predictor.

In the rest of the chapter, the SVMs have a **radial basis function (RBF)** kernel. They are nonlinear, but with smooth separating surfaces. In practice, SVMs work well with many datasets and thus are an integral part of the `scikit-learn` library.

Classifying data with a linear SVM

In the first chapter, we saw some examples of classification with SVMs. We focused on SVMs' slightly superior classification performance compared to logistic regression, but for the most part, we left SVMs alone.

Here, we will focus on them more closely. While SVMs do not have an easy probabilistic interpretation, they do have an easy visual-geometric one. The main idea behind linear SVMs is to separate two classes with the best possible plane.

Let's linearly separate two classes with an SVM.

Getting ready

Let us start by loading and visualizing the iris dataset available in scikit-learn:

Load the data

Load part of the iris dataset. This will allow for easy comparison with the first chapter:

```
#load the libraries we have been using
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt #Library for visualization

from sklearn import datasets

iris = datasets.load_iris()
X_w = iris.data[:, :2] #load the first two features of the iris data
y_w = iris.target      #load the target of the iris data
```

Now, we will use a NumPy mask to focus on the first two classes:

```
#select only the first two classes for both the feature set and target set
#the first two classes of the iris dataset: Setosa (0), Versicolour (1)

X = X_w[y_w < 2]
y = y_w[y_w < 2]
```

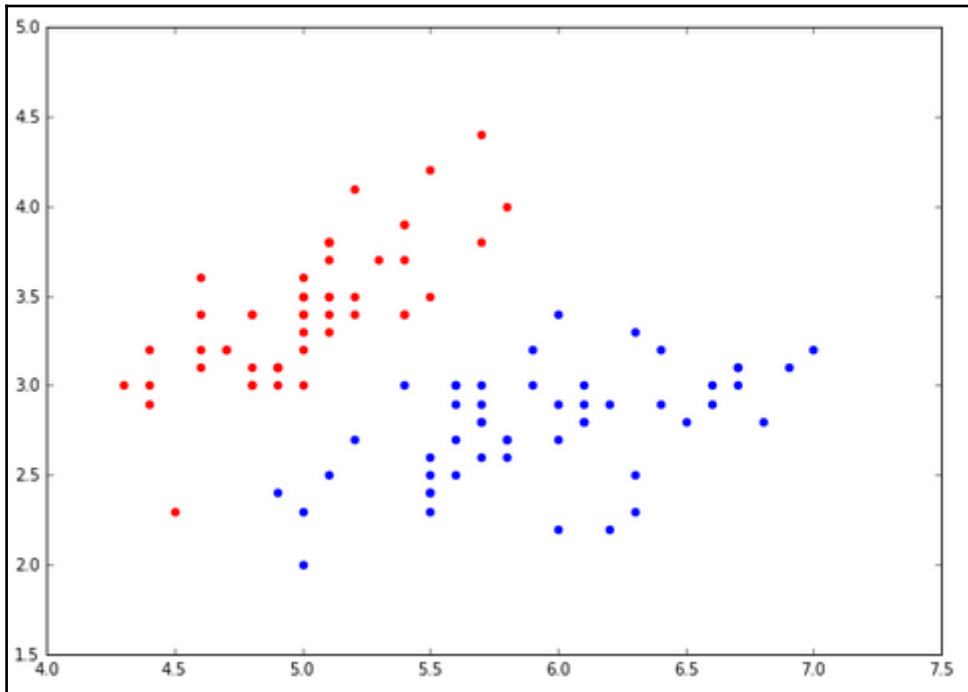
Visualize the two classes

Plot the classes 0 and 1 with matplotlib. Recall that the notation `X_0[:, 0]` refers to the first column of a NumPy array.

In the following code, `X_0` refers to the subset of inputs `x` that correspond to the target `y` being 0 and `X_1` is a subset with a matching target value of 1:

```
X_0 = X[y == 0]
X_1 = X[y == 1]
```

```
#to visualize within IPython:  
%matplotlib inline  
plt.figure(figsize=(10,7)) #change figure-size for easier viewing  
plt.scatter(X_0[:,0],X_0[:,1], color = 'red')  
plt.scatter(X_1[:,0],X_1[:,1], color = 'blue')
```



From the graph, it is clear that we could find a straight line to separate these two classes.

How to do it...

The process of finding the SVM line is straightforward. It is the same process as with any scikit-learn supervised learning estimator:

1. Create training and testing sets.
2. Create an SVM model instance.
3. Fit the SVM model to the loaded data.
4. Predict with the SVM model and measure the performance of the model in preparation for predictions of unseen data.

Let's begin:

1. Split the dataset of the first two features of the first two classes. Stratify the target set:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=7, stratify=y)
```

2. Create an SVM model instance. Set the kernel to be linear, as we want a line to separate the two classes that are involved in this example:

```
from sklearn.svm import SVC

svm_inst = SVC(kernel='linear')
```

3. Fit the model (train the model):

```
svm_inst.fit(X_train, y_train)
```

4. Predict using the test set:

```
y_pred = svm_inst.predict(X_test)
```

5. Measure the performance of the SVM on the test set:

```
from sklearn.metrics import accuracy_score

accuracy_score(y_test, y_pred)

1.0
```

It did perfectly on the test set. This is not surprising, because when we visualized each class, they were easy to visually separate.

6. Visualize the decision boundary, the line separating the classes, by using the estimator on a two-dimensional grid:

```
from itertools import product

#Minima and maxima of both features
xmin, xmax = np.percentile(X[:, 0], [0, 100])
ymin, ymax = np.percentile(X[:, 1], [0, 100])

#Grid/Cartesian product with itertools.product
test_points = np.array([[xx, yy] for xx, yy in
product(np.linspace(xmin, xmax), np.linspace(ymin, ymax))])
```

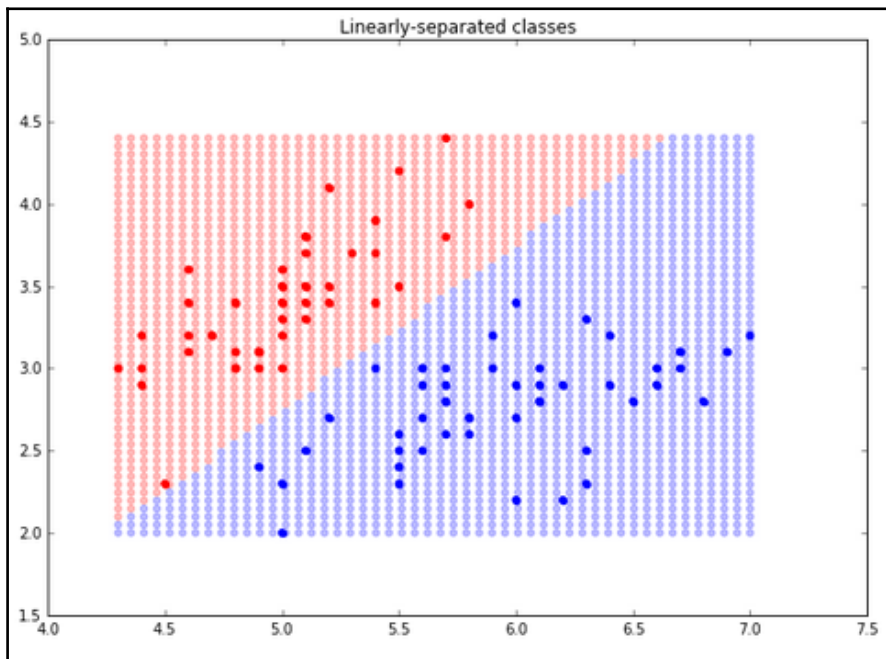
```
#Predictions on the grid
test_preds = svm_inst.predict(test_points)
```

7. Plot the grid by coloring the predictions. Note that we have amended the previous visualization to include SVM predictions:

```
X_0 = X[y == 0]
X_1 = X[y == 1]

%matplotlib inline
plt.figure(figsize=(10,7)) #change figure-size for easier viewing
plt.scatter(X_0[:,0],X_0[:,1], color = 'red')
plt.scatter(X_1[:,0],X_1[:,1], color = 'blue')

colors = np.array(['r', 'b'])
plt.scatter(test_points[:, 0], test_points[:, 1],
            color=colors[test_preds], alpha=0.25)
plt.scatter(X[:, 0], X[:, 1], color=colors[y])
plt.title("Linearly-separated classes")
```



We fleshed out the SVM linear decision boundary by predicting on a two-dimensional grid.

How it works...

At times, it could be computationally expensive to predict on a whole grid of points, especially if the SVM is predicting many classes in many dimensions. In these cases, you will need access to the geometric information of the SVM decision boundary.

A linear decision boundary, a hyperplane, is uniquely specified by a vector normal to the hyperplane and an intercept. The normal vectors are contained in the SVM instance's `coef_` data attribute. The intercepts are contained in the SVM instance's `intercept_` data attribute. View these two attributes:

```
svm_inst.coef_
array([[ 2.22246001, -2.2213921 ]])

svm_inst.intercept_
array([-5.00384439])
```

You might be able to quickly see that the `coef_[0]` vector is perpendicular to the line we drew to separate both of the iris classes we have been viewing.

Every time, these two NumPy arrays, `svm_inst.coef_` and `svm_inst.intercept_`, will have the same number of rows. Each row corresponds to each plane separating the classes involved. In the example, there are two classes linearly separated by one hyperplane. The particular SVM type, SVC in this case, implements a one-versus-one classifier: it will draw a unique plane separating every pair of classes involved.

If we were trying to separate three classes, there would be three possible combinations, $3 \times 2/2 = 3$. For n classes, the number of planes provided by SVC is as follows:

$$\text{Number of planes} = \frac{\text{Number of classes} \times (\text{Number of classes} - 1)}{2}$$

The number of columns in the `coef_` data attribute is the number of features in the data, which in this case is two.

To find the decision in regards to a point in space, solve the following equation for zero:

<p>When...</p> <p>coef_array C</p> <p>A vector in space</p> <p>intercept_vector \vec{i}</p>	$C\vec{v} + \vec{i}$ <p>denotes \vec{v}'s location relative to the decision boundary</p>
Thus...	
$C\vec{v} + \vec{i} > 0$	Vector v is on one side of the hyperplane
$C\vec{v} + \vec{i} = 0$	Vector v is on the hyperplane
$C\vec{v} + \vec{i} < 0$	Vector v is on the other side of the hyperplane

If you only desire the uniqueness of the plane, store the tuple (coef_, intercept_).

There's more...

Additionally, you can view the the parameters of the instance to learn more about it:

```
svm_inst
```

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape=None, degree=3, gamma='auto', kernel='linear',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
```

Traditionally, the SVC prediction performance is optimized over the following parameters: C , γ , and the shape of the kernel. C describes the margin of the SVM and is set to one by default. The margin is the empty space on either side of the hyperplane with no class examples. If your dataset has many noisy observations, try higher C s with cross-validation. C is proportional to error on the margin, and as C gets higher in value, the SVM will try to make the margin smaller.

A final note on SVMs is that we could re-scale the data and test that scaling with cross-validation. Conveniently, the iris dataset has units of cms for all of the inputs so re-scaling is not necessary but for an arbitrary dataset you should look into it.

Optimizing an SVM

For this example we will continue with the iris dataset, but will use two classes that are harder to tell apart, the Versicolour and Virginica iris species.

In this section we will focus on the following:

- **Setting up a scikit-learn pipeline:** A chain of transformations with a predictive model at the end
- **A grid search:** A performance scan of several versions of SVMs with varying parameters

Getting ready

Load two classes and two features of the iris dataset:

```
#load the libraries we have been using
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn import datasets

iris = datasets.load_iris()
X_w = iris.data[:, :2] #load the first two features of the iris data
y_w = iris.target      #load the target of the iris data

X = X_w[y_w != 0]
y = y_w[y_w != 0]

X_1 = X[y == 1]
X_2 = X[y == 2]
```

How to do it...

1. Begin by splitting the data into training and testing sets:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, random_state=7, stratify=y)
```

Construct a pipeline

2. Then construct a pipeline with two steps: a scaling step and an SVM step. It is best to scale the data before passing it to an SVM:

```
from sklearn.svm import SVC
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

svm_est = Pipeline([('scaler', StandardScaler()), ('svc', SVC())])
```



Note that in the pipeline, the scaling step has the name `scaler` and the SVM has the name `svc`. The names will be crucial in the next step. Note that the default SVM is an RBF SVM, which is nonlinear.

Construct a parameter grid for a pipeline

3. Vary the relevant RBF parameters, `C` and `gamma`, logarithmically, varying by one order of magnitude at a time:

```
Cs = [0.001, 0.01, 0.1, 1, 10]
gammas = [0.001, 0.01, 0.1, 1, 10]
```

4. Finally, construct the parameter grid by making it into a dictionary. The SVM parameter dictionary key names begin with `svc__`, taking the pipeline SVM name and adding two underscores. This is followed by the parameter name within the SVM estimator, `C` and `gamma`:

```
param_grid = dict(svc__gamma=gammas, svc__C=Cs)
```

Provide a cross-validation scheme

5. The following is a stratified and shuffled split. The `n_splits` parameter refers to the number of splits, or tries, the dataset will be split into. The `test_size` parameter is how much data will be left out for testing within the fold. The estimator will be scored using the test set on each fold:

```
from sklearn.model_selection import StratifiedShuffleSplit

cv = StratifiedShuffleSplit(n_splits=5, test_size=0.2,
                             random_state=7)
```

The most important element of the stratified shuffle is that each fold preserves the proportion of samples for each class.

6. For a plain cross-validation scheme, set `cv` to an integer representing the number of folds:

```
cv = 10
```

Perform a grid search

There are three required elements for a grid search:

- An estimator
- A parameter grid
- A cross-validation scheme

7. We have those three elements. Set up the grid search. Run it on the training set:

```
from sklearn.model_selection import GridSearchCV

grid_cv = GridSearchCV(svm_est, param_grid=param_grid, cv=cv)
grid_cv.fit(X_train, y_train)
```

8. Look up the best parameters found with the grid search:

```
grid_cv.best_params_

{'svc__C': 10, 'svc__gamma': 0.1}
```

9. Look up the best score, that pertains to the best estimator:

```
grid_cv.best_score_  
  
0.71250000000000002
```

There's more...

Let us look at additional perspectives of SVM for classification.

Randomized grid search alternative

scikit-learn's `GridSearchCV` performs a full scan for the best set of parameters for the estimator. In this case, it searches the $5 \times 5 = 25$ (C, gamma) pairs specified by the `param_grid` parameter.

An alternative would have been using `RandomizedSearchCV`, by using the following line instead of the one used with `GridSearchCV`:

```
from sklearn.model_selection import RandomizedSearchCV  
  
rand_grid = RandomizedSearchCV(svm_est, param_distributions=param_grid,  
cv=cv, n_iter=10)  
rand_grid.fit(X_train, y_train)
```

It yields the same C and gamma:

```
rand_grid.best_params_  
  
{'svc__C': 10, 'svc__gamma': 0.001}
```

Visualize the nonlinear RBF decision boundary

Visualize the RBF decision boundary with code similar to the previous recipe. First, create a grid and predict to which class each point on the grid corresponds:

```
from itertools import product  
  
#Minima and maxima of both features  
xmin, xmax = np.percentile(X[:, 0], [0, 100])  
ymin, ymax = np.percentile(X[:, 1], [0, 100])  
  
#Grid/Cartesian product with itertools.product
```

```
test_points = np.array([[xx, yy] for xx, yy in product(np.linspace(xmin,
xmax), np.linspace(ymin, ymax))])

#Predictions on the grid
test_preds = grid_cv.predict(test_points)
```

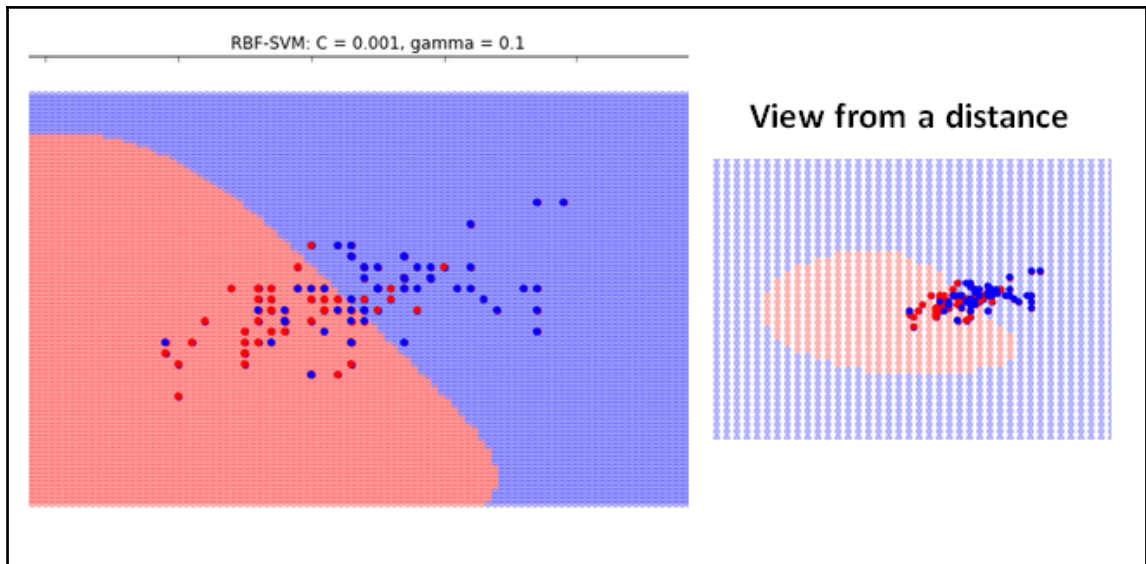
Now visualize the grid:

```
X_1 = X[y == 1]
X_2 = X[y == 2]

%matplotlib inline
plt.figure(figsize=(10,7)) #change figure-size for easier viewing
plt.scatter(X_2[:,0],X_2[:,1], color = 'red')
plt.scatter(X_1[:,0],X_1[:,1], color = 'blue')

colors = np.array(['r', 'b'])
plt.scatter(test_points[:, 0], test_points[:, 1],
color=colors[test_preds-1], alpha=0.25)
plt.scatter(X[:, 0], X[:, 1], color=colors[y-1])
plt.title("RBF-separated classes")
```

Note that in the resulting graph, the RBF curve looks quite straight, but it really corresponds to a slight curve. This is an SVM with $\gamma = 0.1$ and $C = 0.001$:



More meaning behind C and gamma

More intuitively, the gamma parameter determines how influential a single example can be per units of distance. If gamma is low, examples have an influence at long distances. If gamma is high, their influence is only over short distances. The SVM selects support vectors in its implementation, and gamma is inversely proportional to the radius of influence of these vectors.

With regard to C, a low C makes the decision surface smoother, while a high C makes the SVM try to classify all the examples correctly and leads to surfaces that are not as smooth.

Multiclass classification with SVM

We begin expanding the previous recipe to classify all iris flower types based on two features. This is not a binary classification problem, but a multiclass classification problem. These steps expand on the previous recipe.

Getting ready

The SVC classifier (scikit's SVC) can be changed slightly in the case of multiclass classifications. For this, we will use all three classes of the iris dataset.

Load two features for each class:

```
#load the libraries we have been using
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn import datasets

iris = datasets.load_iris()
X = iris.data[:, :2] #load the first two features of the iris data
y = iris.target      #load the target of the iris data

X_0 = X[y == 0]
X_1 = X[y == 1]
X_2 = X[y == 2]
```


Split the data into training and testing sets:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
random_state=7, stratify=y)
```

How to do it...

OneVsRestClassifier

1. Load `OneVsRestClassifier` within a pipeline:

```
from sklearn.svm import SVC
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.multiclass import OneVsRestClassifier

svm_est =
Pipeline([('scaler', StandardScaler()), ('svc', OneVsRestClassifier(SVC()))])
```

2. Set up a parameter grid:

```
Cs = [0.001, 0.01, 0.1, 1, 10]
gammas = [0.001, 0.01, 0.1, 1, 10]
```

3. Construct the parameter grid. Note the very special syntax to denote the `OneVsRestClassifier` SVC. The parameter key names within the dictionary start with `svc__estimator__` when named `svc` within the pipeline:

```
param_grid = dict(svc__estimator__gamma=gammas,
svc__estimator__C=Cs)
```

4. Load a randomized hyperparameter search. Fit it:

```
from sklearn.model_selection import RandomizedSearchCV
from sklearn.model_selection import StratifiedShuffleSplit

cv = StratifiedShuffleSplit(n_splits=5, test_size=0.2,
                             random_state=7)
rand_grid = RandomizedSearchCV(svm_est,
                                param_distributions=param_grid, cv=cv, n_iter=10)
rand_grid.fit(X_train, y_train)
```

5. Look up the best parameters:

```
rand_grid.best_params_

{'svc__estimator__C': 10, 'svc__estimator__gamma': 0.1}
```

Visualize it

We are going to predict the category of every point in a two-dimensional grid by calling the trained SVM to predict along the grid:

```
%matplotlib inline
from itertools import product

#Minima and maxima of both features
xmin, xmax = np.percentile(X[:, 0], [0, 100])
ymin, ymax = np.percentile(X[:, 1], [0, 100])

#Grid/Cartesian product with itertools.product
test_points = np.array([[xx, yy] for xx, yy in product(np.linspace(xmin,
                                                                    xmax, 100),
                                                         np.linspace(ymin,
                                                                    ymax, 100))])

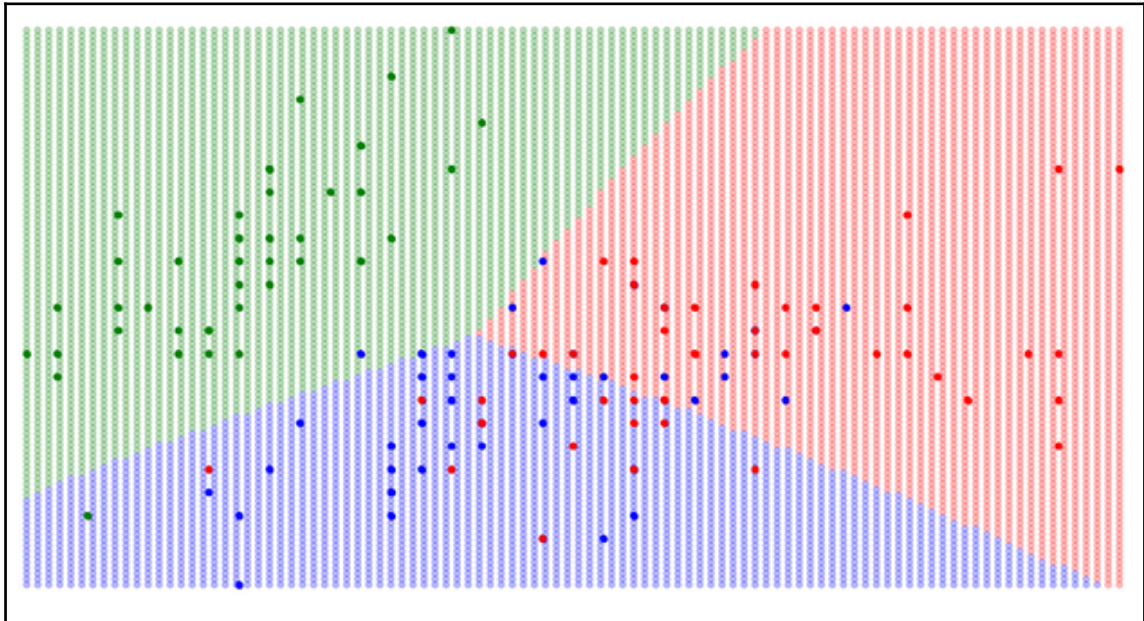
#Predictions on the grid
test_preds = rand_grid.predict(test_points)

plt.figure(figsize=(15,9))    #change figure-size for easier viewing

plt.scatter(X_0[:,0],X_0[:,1], color = 'green')
plt.scatter(X_1[:,0],X_1[:,1], color = 'blue')
plt.scatter(X_2[:,0],X_2[:,1], color = 'red')

colors = np.array(['g', 'b', 'r'])
plt.tight_layout()
plt.scatter(test_points[:, 0], test_points[:, 1], color=colors[test_preds],
```

```
alpha=0.25)  
plt.scatter(X[:, 0], X[:, 1], color=colors[y])
```



The boundaries generated by SVM tend to be smooth curves, very different from the tree-based boundaries we will see in upcoming chapters.

How it works...

The `OneVsRestClassifier` creates many binary SVC classifiers: one for each class versus the rest of the classes. In this case, three decision boundaries will be computed because there are three classes. This type of classifier is easy to conceptualize because there are fewer decision boundaries and surfaces.

If there were 10 classes, there would be $10 \times 9/2 = 45$ surfaces if SVC was the default `OneVsOneClassifier`. On the other hand, there would be 10 surfaces for the `OneVsAllClassifier`.

Support vector regression

We will capitalize on the SVM classification recipes by performing support vector regression on scikit-learn's diabetes dataset.

Getting ready

Load the diabetes dataset:

```
#load the libraries we have been using
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn import datasets

diabetes = datasets.load_diabetes()

X = diabetes.data
y = diabetes.target
```

Split the data in training and testing sets. There is no stratification for regression in this case:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
random_state=7)
```

How to do it...

1. Create a `OneVsRestClassifier` within a pipeline and **support vector regression (SVR)** from `sklearn.svm`:

```
from sklearn.svm import SVR
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.multiclass import OneVsRestClassifier

svm_est =
Pipeline([('scaler', StandardScaler()), ('svc', OneVsRestClassifier(SV
R()))])
```

2. Create a parameter grid:

```
Cs = [0.001, 0.01, 0.1, 1]
gammas = [0.001, 0.01, 0.1]

param_grid = dict(svc__estimator__gamma=gammas,
                  svc__estimator__C=Cs)
```

3. Perform a randomized search of the best hyperparameters, C and gamma:

```
from sklearn.model_selection import RandomizedSearchCV
from sklearn.model_selection import StratifiedShuffleSplit

rand_grid = RandomizedSearchCV(svm_est,
                               param_distributions=param_grid,
                               cv=5, n_iter=5, scoring='neg_mean_absolute_error')
rand_grid.fit(X_train, y_train)
```

4. Look at the best parameters:

```
rand_grid.best_params_

{'svc__estimator__C': 10, 'svc__estimator__gamma': 0.1}
```

5. Look at the best score:

```
rand_grid.best_score_

-58.059490084985839
```

The score does not seem very good. Try different algorithms with different score setups and see which one performs best.

9

Tree Algorithms and Ensembles

In this chapter we will cover the following recipes:

- Doing basic classifications with decision trees
- Visualizing a decision tree with pydot
- Tuning a decision tree
- Using decision trees for regression
- Reducing overfitting with cross-validation
- Implementing random forest regression
- Bagging regression with nearest neighbor
- Tuning gradient boosting trees
- Tuning an AdaBoost regressor
- Writing a stacking aggregator with scikit-learn

Introduction

In this chapter, we focus on decision trees and ensemble algorithms. Decision algorithms are easy to interpret and visualize as they are outlines of the decision making process we are familiar with. Ensembles can be partially interpreted and visualized, but they have many parts (base estimators), so we cannot always read them easily.

The goal of ensemble learning is that several estimators can work better than a single one. There are two families of ensemble methods implemented in scikit-learn: averaging methods and boosting methods. Averaging methods (random forest, bagging, extra trees) reduce variance by averaging the predictions of several estimators. Boosting methods (gradient boost and AdaBoost) reduce bias by sequential building base estimators with the goal of reducing the bias of the whole ensemble.

A common characteristic of many ensemble constructions is using randomness to build predictors. Random forest, for example, uses randomness (as its name implies), and we will use a search through many model parameters using randomness. Use the ideas of randomness in this chapter to build on them at work, reduce the computational cost, and produce better-scoring algorithms.

We finish the chapter with a stacking aggregator, which is an ensemble of potentially very different models. Part of the data analysis in stacking is taking predictions of several machine learning algorithms as input.



A lot of data science is computationally intensive. If possible, use a multi-core computer. Throughout, there is a parameter called `n_jobs` set to `-1`, which utilizes all of your computer's cores.

Doing basic classifications with decision trees

Here, we perform basic classification with decision trees. Decision trees for classification are sequences of decisions that determine a classification, or a categorical outcome. Additionally, the decision tree can be examined in SQL by other individuals within the same company looking at the data.

Getting ready

Start by loading the iris dataset once again and dividing the data into training and testing sets:

```
from sklearn.datasets import load_iris

iris = load_iris()

X = iris.data
```

```
y = iris.target

from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
stratify=y)
```

How to do it...

1. Import the decision tree classifier and train it on the training set:

```
from sklearn.tree import DecisionTreeClassifier

dtc = DecisionTreeClassifier()      #Instantiate tree class
dtc.fit(X_train, y_train)
```

2. Then measure the accuracy on the test set:

```
from sklearn.metrics import accuracy_score

y_pred = dtc.predict(X_test)
accuracy_score(y_test, y_pred)

0.911111111111111109
```

The decision tree appears to be accurate. Let's examine it further.

Visualizing a decision tree with pydot

If you would like to produce graphs, install the `pydot` library. Unfortunately, for Windows this installation could be non-trivial. Please focus on looking at the graphs rather than reproducing them if you struggle to install `pydot`.

How to do it...

1. Within an IPython Notebook, perform several imports and type the following script:

```
import numpy as np
from sklearn import tree
from sklearn.externals.six import StringIO
```

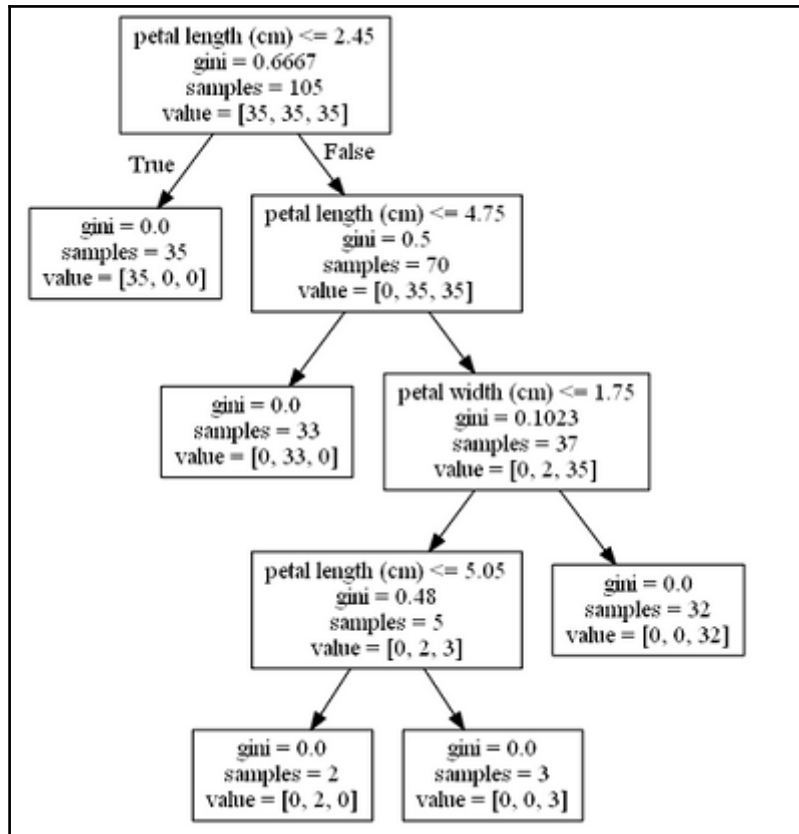


```

import pydot
from IPython.display import Image

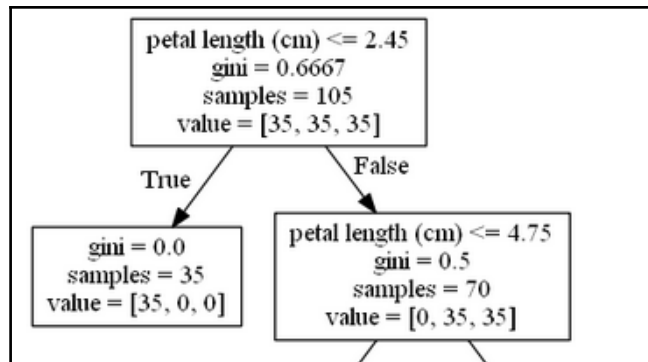
dot_iris = StringIO()
tree.export_graphviz(dtc, out_file = dot_iris, feature_names =
iris.feature_names)
graph = pydot.graph_from_dot_data(dot_iris.getvalue())
Image(graph.create_png())

```



How it works...

This is the decision tree that was produced with the training; calling the `fit` method on `x_train` and `y_train`. Look at it closely, starting at the top of the tree. You have 105 samples in the training set. The training set is split into three sets of 35 each: *value* = [35, 35, 35]. Explicitly, these are 35 Setosa, 35 Versicolor, and 35 Virginica flowers:



The first decision is whether the petal length of the flower is less than or equal to 2.45. If the answer is true, or yes, the flower is classified as being in the first category, *value* = [35, 0, 0]. The flower is classified as being a Setosa flower. In several examples of the iris dataset classification, this one was the easiest to classify.

Otherwise, if the petal length is greater than 2.45, the first decision leads to a smaller decision tree. The smaller decision tree only has flowers of the last two types, Versicolour and Virginica, and the *value* = [0, 35, 35].

The algorithm proceeds to produce a complete tree of four levels, depth 4 (note that the top node is not included in counting the levels). With formal language, the three nodes characterizing a decision in the picture are called a **split**.

There's more...

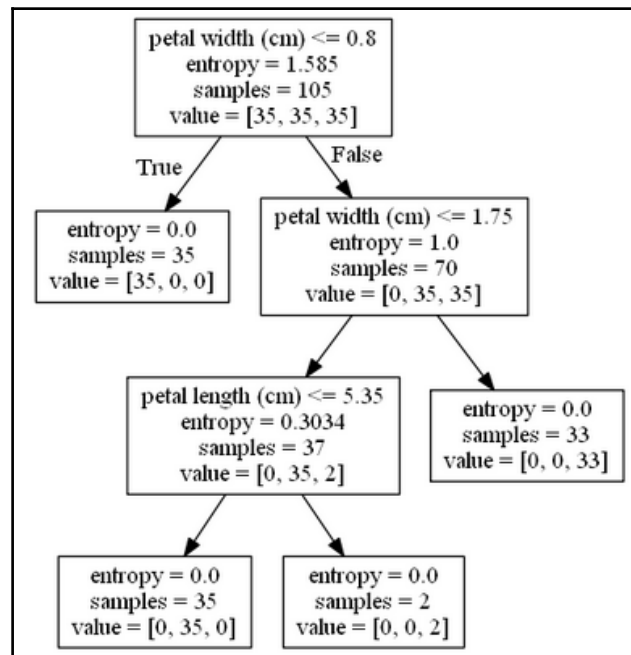
You might wonder what the gini reference is within the visualization of the decision tree. Gini refers to the gini function, which measures the quality of a split, with three nodes representing a decision. When the algorithm runs, a few splits that optimize the gini function are considered. The split that produces the best gini impurity measure is chosen.

Another option is to measure entropy to determine how to split the tree. You can try both options and determine which is best using cross-validation. Change the criterion in the decision tree as follows:

```
from sklearn.tree import DecisionTreeClassifier

dtt = DecisionTreeClassifier(criterion='entropy')
dtt.fit(X_train, y_train)
```

This leads to the following diagram of the tree:



You can examine how this criterion performs under cross-validation using `GridSearchCV` and vary the criterion parameter in the parameter grid. We will do this in the next section.

Tuning a decision tree

We will continue to explore the iris dataset further by focusing on the first two features (sepal length and sepal width), optimizing the decision tree, and creating some visualizations.

Getting ready

1. Load the iris dataset, focusing on the first two features. Additionally, split the data into training and testing sets:

```
from sklearn.datasets import load_iris

iris = load_iris()
X = iris.data[:, :2]
y = iris.target

from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.3, stratify=y)
```

2. View the data with pandas:

```
import pandas as pd
pd.DataFrame(X, columns=iris.feature_names[:2])
```

	sepal length (cm)	sepal width (cm)
0	5.1	3.5
1	4.9	3.0
2	4.7	3.2
3	4.6	3.1
4	5.0	3.6
5	5.4	3.9
6	4.6	3.4
7	5.0	3.4
8	4.4	2.9

3. Before optimizing the decision tree, let's try a single decision tree with default parameters. Instantiate and train a decision tree:

```
from sklearn.tree import DecisionTreeClassifier

dtc = DecisionTreeClassifier()    #Instantiate tree with default
parameters
dtc.fit(X_train, y_train)
```

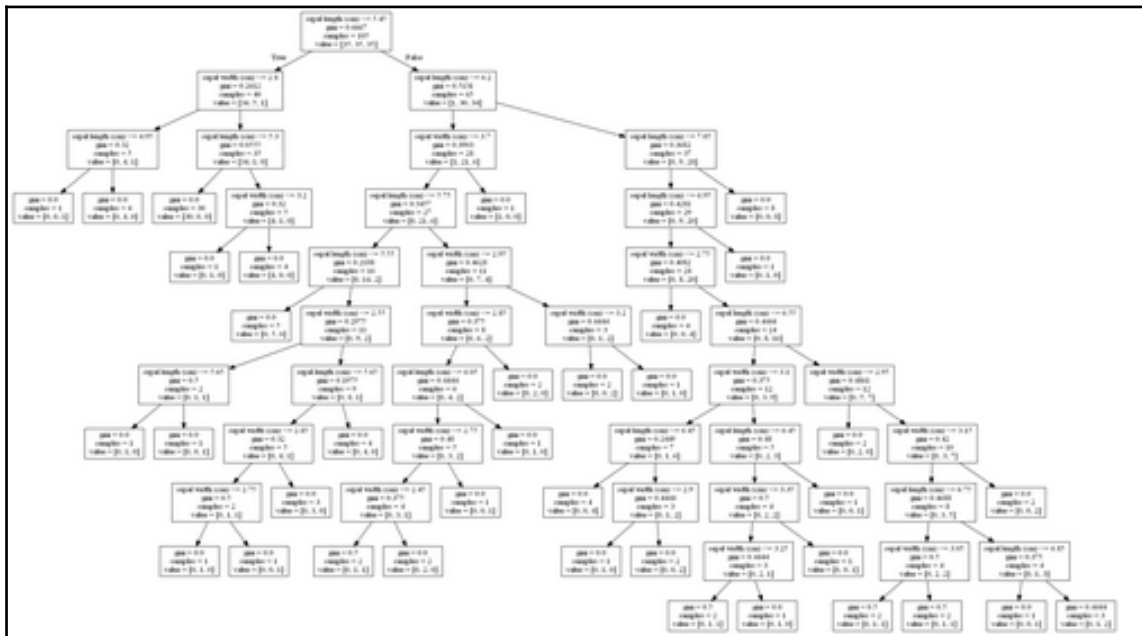
4. Measure the accuracy score:

```
from sklearn.metrics import accuracy_score

y_pred = dtc.predict(X_test)
accuracy_score(y_test, y_pred)

0.6666666666666663
```

Visualizing the tree with `graphviz` reveals a very complex tree with many nodes and levels (the image is for representational purposes only: it is OK if you cannot read it! It is a very deep tree with lots of overfitting!):



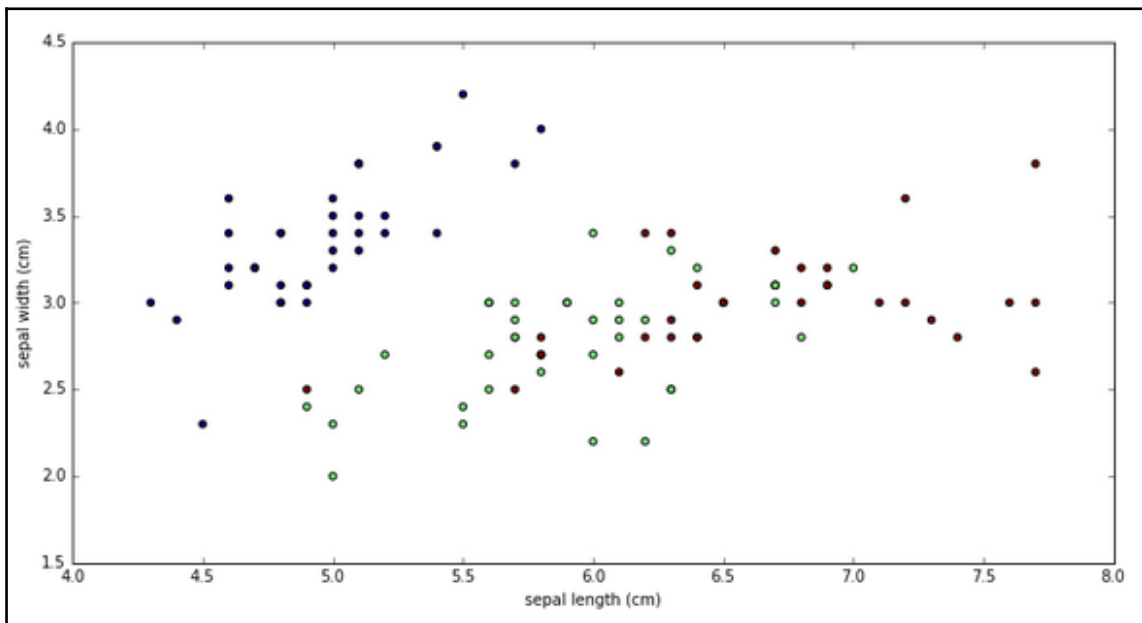
This is a case of overfitting. The decision tree is very elaborate. The whole iris dataset consists of 150 samples, and a very complex tree is undesirable. Recall that in previous chapters we have used linear SVMs, which split space in a simple way with a few straight lines.

Before continuing, visualize the training data points using matplotlib:

```
import matplotlib.pyplot as plt
%matplotlib inline

plt.figure(figsize=(12,6))
plt.xlabel(iris.feature_names[0])
plt.ylabel(iris.feature_names[1])

plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train)
```



How to do it...

1. To optimize the decision tree's performance, use `GridSearchCV`. Start by instantiating a decision tree:

```
from sklearn.tree import DecisionTreeClassifier
dtc = DecisionTreeClassifier()
```

2. Then, instantiate and train `GridSearchCV`:

```
from sklearn.model_selection import GridSearchCV, cross_val_score

param_grid = {'criterion': ['gini', 'entropy'], 'max_depth' :
              [3, 5, 7, 20]}

gs_inst = GridSearchCV(dtc, param_grid=param_grid, cv=5)
gs_inst.fit(X_train, y_train)
```



Note how in the parameter grid, `param_grid`, we vary the split scoring criterion between `gini` and `entropy` and vary the `max_depth` of a tree.

3. Now try to score the accuracy on the test set:

```
from sklearn.metrics import accuracy_score

y_pred_gs = gs_inst.predict(X_test)
accuracy_score(y_test, y_pred_gs)

0.6888888888888888
```

The accuracy improved slightly. Let's look at `GridSearchCV` more closely.

4. View the scores of all the decision trees tried in the grid search:

```
gs_inst.grid_scores_

[mean: 0.78095, std: 0.09331, params: {'criterion': 'gini',
'max_depth': 3},
 mean: 0.68571, std: 0.08832, params: {'criterion': 'gini',
'max_depth': 5},
 mean: 0.70476, std: 0.08193, params: {'criterion': 'gini',
'max_depth': 7},
 mean: 0.66667, std: 0.09035, params: {'criterion': 'gini',
'max_depth': 20},
```

```

    mean: 0.78095, std: 0.09331, params: {'criterion': 'entropy',
'max_depth': 3},
    mean: 0.69524, std: 0.11508, params: {'criterion': 'entropy',
'max_depth': 5},
    mean: 0.72381, std: 0.09712, params: {'criterion': 'entropy',
'max_depth': 7},
    mean: 0.67619, std: 0.09712, params: {'criterion': 'entropy',
'max_depth': 20}]

```



Note that this method will be unavailable in future versions of scikit-learn. Feel free to use

```
zip(gs_inst.cv_results_['mean_test_score'], gs_inst.cv_results_['params'])
```

to produce similar results.

From this list of scores, you can see that deeper trees perform worse than shallow trees. In detail, the data in the training set is split into five parts. Training occurs in four parts while testing happens in one of the five parts. Very deep trees overfit: they perform well on the training sets, but on the five testing sets of the cross-validation, they perform badly.

5. Select the best performing tree with the `best_estimator_` attribute:

```

gs_inst.best_estimator_

DecisionTreeClassifier(class_weight=None, criterion='gini',
max_depth=3,
    max_features=None, max_leaf_nodes=None,
    min_impurity_split=1e-07, min_samples_leaf=1,
    min_samples_split=2, min_weight_fraction_leaf=0.0,
    presort=False, random_state=None, splitter='best')

```

6. Visualize the tree with `graphviz`:

```

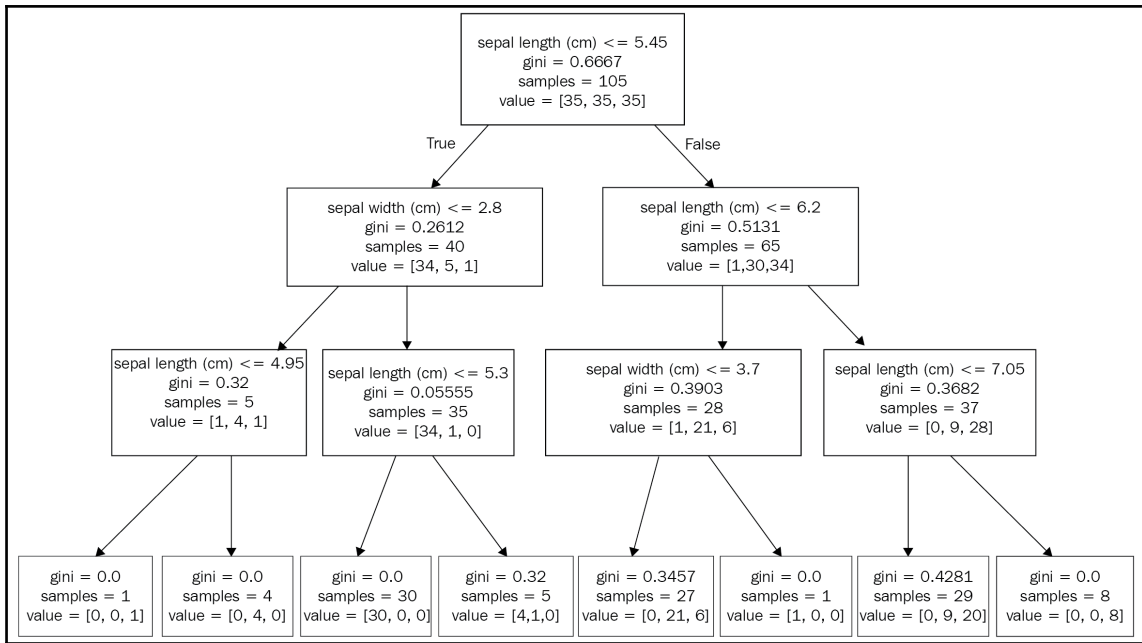
import numpy as np
from sklearn import tree
from sklearn.externals.six import StringIO

import pydot
from IPython.display import Image

dot_iris = StringIO()
tree.export_graphviz(gs_inst.best_estimator_, out_file = dot_iris,
    feature_names = iris.feature_names[:2])
graph = pydot.graph_from_dot_data(dot_iris.getvalue())

Image(graph.create_png())

```

There's more...

1. For additional insight, we will create an additional visualization. Start by creating a NumPy mesh grid as follows:

```

grid_interval = 0.02

x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5

xmin, xmax = np.percentile(X[:, 0], [0, 100])
ymin, ymax = np.percentile(X[:, 1], [0, 100])

xmin_plot, xmax_plot = xmin - .5, xmax + .5
ymin_plot, ymax_plot = ymin - .5, ymax + .5

xx, yy = np.meshgrid(np.arange(xmin_plot, xmax_plot,
                                grid_interval),
                    np.arange(ymin_plot, ymax_plot, grid_interval))
  
```

2. Using the `best_estimator_` attribute in the grid search, predict the scenarios on the NumPy grid that was just created:

```
test_preds =
gs_inst.best_estimator_.predict(np.array(zip(xx.ravel(),
yy.ravel()))))
```

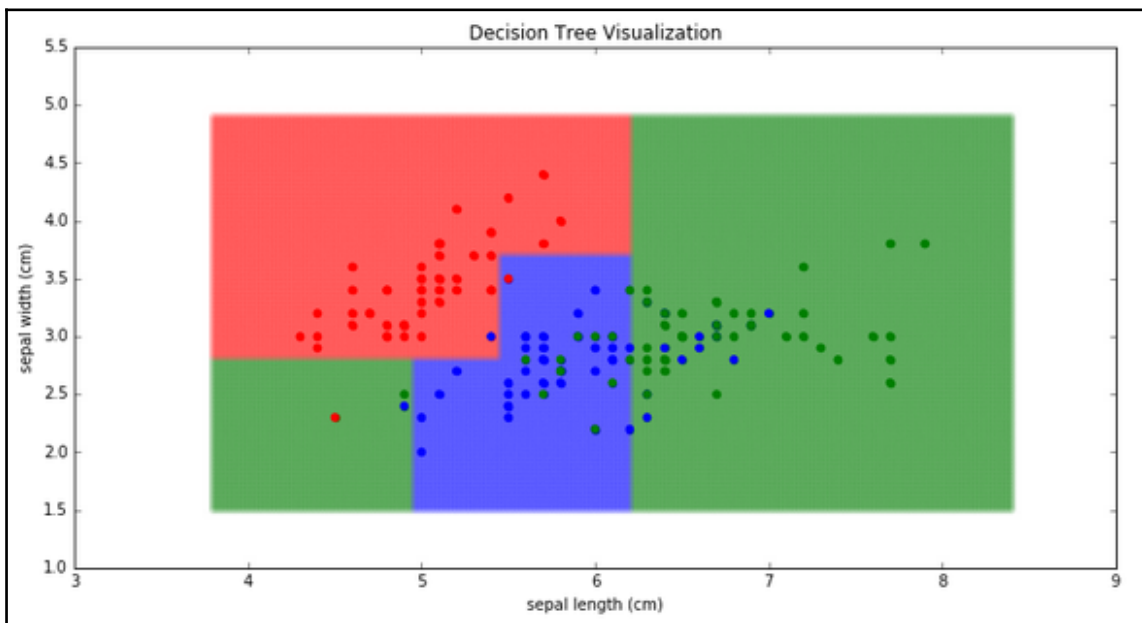
3. Look at the visualization:

```
import matplotlib.pyplot as plt
%matplotlib inline

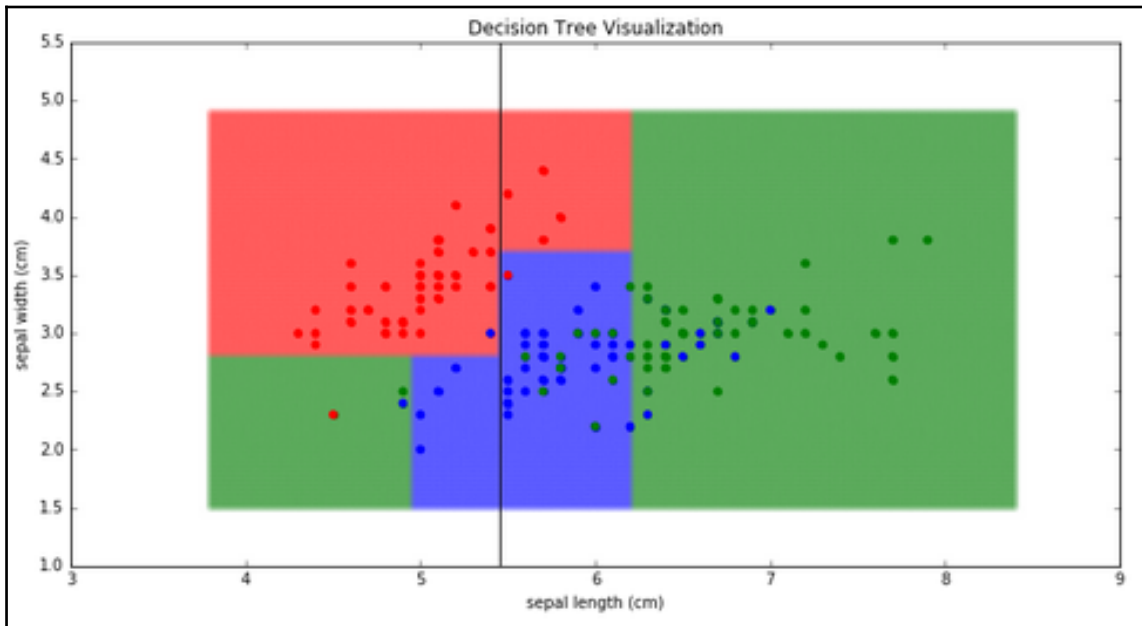
X_0 = X[y == 0]
X_1 = X[y == 1]
X_2 = X[y == 2]

plt.figure(figsize=(15,8)) #change figure-size for easier viewing
plt.scatter(X_0[:,0],X_0[:,1], color = 'red')
plt.scatter(X_1[:,0],X_1[:,1], color = 'blue')
plt.scatter(X_2[:,0],X_2[:,1], color = 'green')

colors = np.array(['r', 'b','g'])
plt.scatter(xx.ravel(), yy.ravel(), color=colors[test_preds],
alpha=0.15)
plt.scatter(X[:, 0], X[:, 1], color=colors[y])
plt.title("Decision Tree Visualization")
plt.xlabel(iris.feature_names[0])
plt.ylabel(iris.feature_names[1])
```

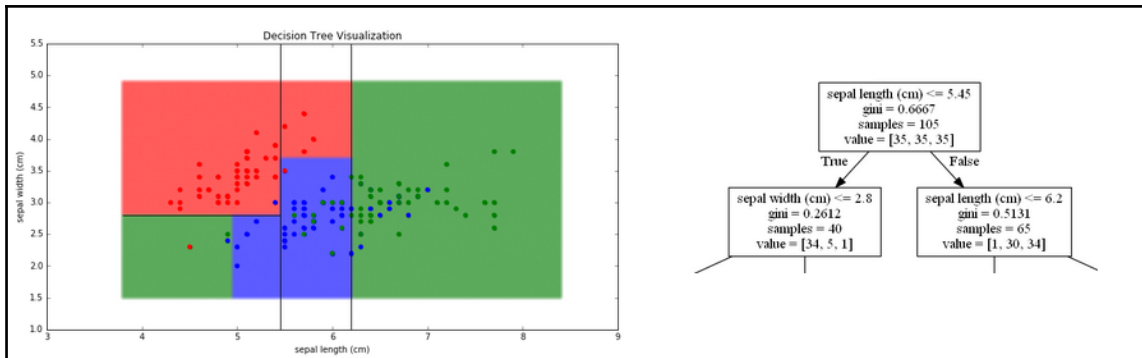


4. Using this type of visualization, you can see that decision trees try to construct rectangles to classify the type of iris flower. Every split creates a line perpendicular to one of the features. In the following graph there is a vertical line depicting the first decision, whether sepal length is greater (right of the line) or less than (left of the line) the number 5.45. Typing `plt.axvline(x = 5.45, color='black')` with the preceding code yields the following result:



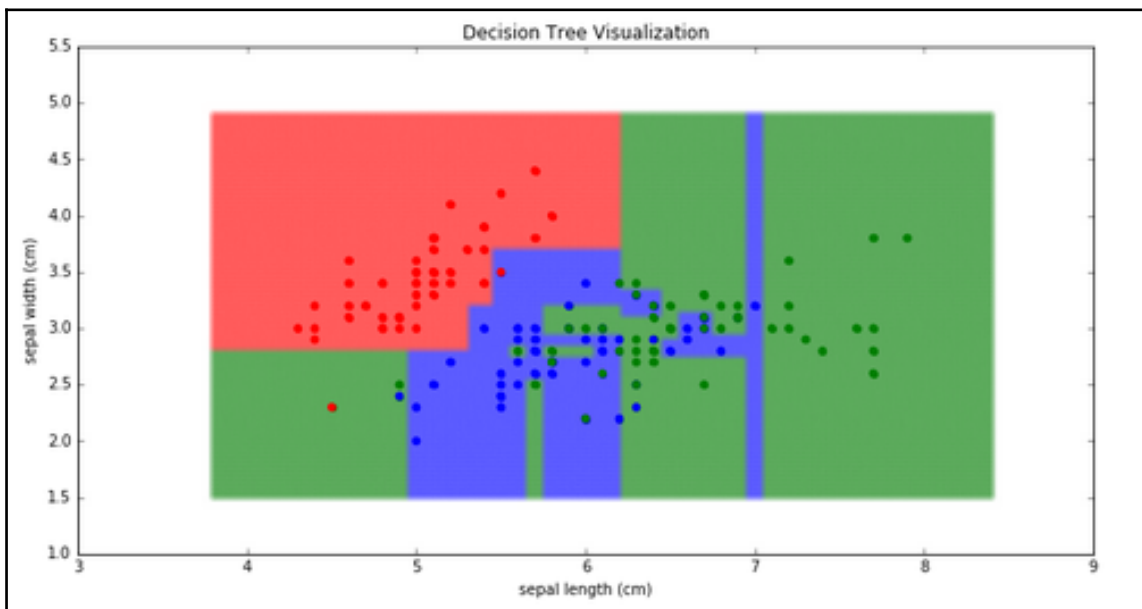
5. Visualize the first three lines:

```
plt.axvline(x = 5.45, color='black')
plt.axvline(x = 6.2, color='black')
plt.plot((xmin_plot, 5.45), (2.8, 2.8), color='black')
```



The horizontal line, $\text{sepal_width} = 2.8$, is shorter and ends at $x = 5.45$ because it does not apply to the case of $\text{sepal_length} \geq 5.45$. In the end, several rectangular regions are created.

6. The following graph shows the same type of visualization applied to the very large decision tree that overfits. The decision tree classifier attempts to place a rectangle around many specific samples of the iris dataset, which shows how it generalizes poorly with new samples:



7. Finally, you could also plot how max depth influences the cross-validation score. Script a grid search with a max depth range from 2 to 51:

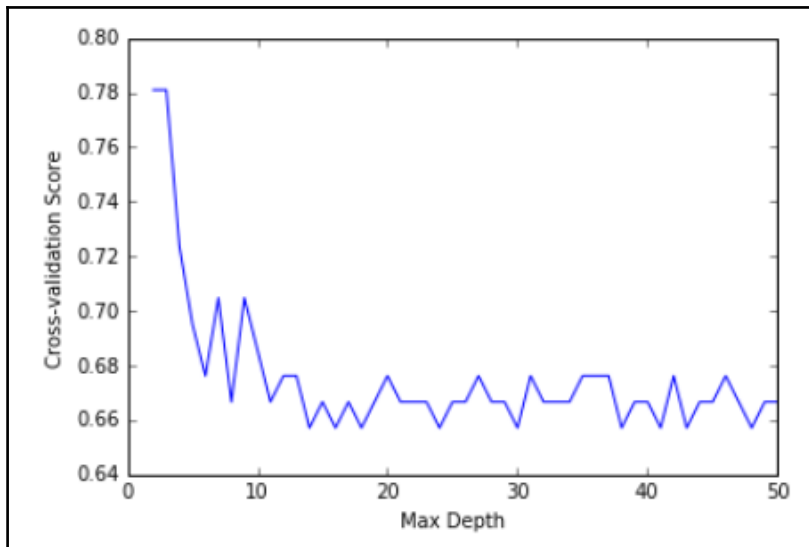
```
from sklearn.tree import DecisionTreeClassifier
dtc = DecisionTreeClassifier()

from sklearn.model_selection import GridSearchCV, cross_val_score

max_depths = range(2, 51)
param_grid = {'max_depth' : max_depths}

gs_inst = GridSearchCV(dtc, param_grid=param_grid, cv=5)
gs_inst.fit(X_train, y_train)

plt.plot(max_depths, gs_inst.cv_results_['mean_test_score'])
plt.xlabel('Max Depth')
plt.ylabel('Cross-validation Score')
```



The plot shows, from a different perspective, that a higher max depth tends to decrease the cross-validation score.

Using decision trees for regression

Decision trees for regression are very similar to decision trees for classification. The procedure for developing a regression model consists of four parts:

- Load the dataset
- Split the set into training/testing subsets
- Instantiate a decision tree regressor and train it
- Score the model on the test subset

Getting ready

For this example, load scikit-learn's diabetes dataset:

```
#Use within an Jupyter notebook
%matplotlib inline

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import load_diabetes

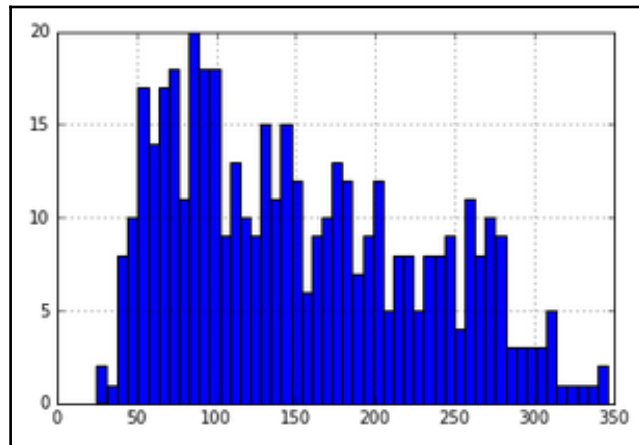
diabetes = load_diabetes()

X = diabetes.data
y = diabetes.target

X_feature_names = ['age', 'gender', 'body mass index', 'average blood
pressure', 'b1_0', 'b1_1', 'b1_2', 'b1_3', 'b1_4', 'b1_5']
```

Now that we have loaded the dataset, we must split the data into training and testing subsets. Before doing that, however, visualize the target variable using pandas:

```
pd.Series(y).hist(bins=50)
```



This is a regression example, and we cannot use `stratify=y` when splitting the dataset. Instead, we will bin the target variable: we will keep track of whether the target variable is less than 50, or between 50 and 100, and so on.

Create bins of width 50:

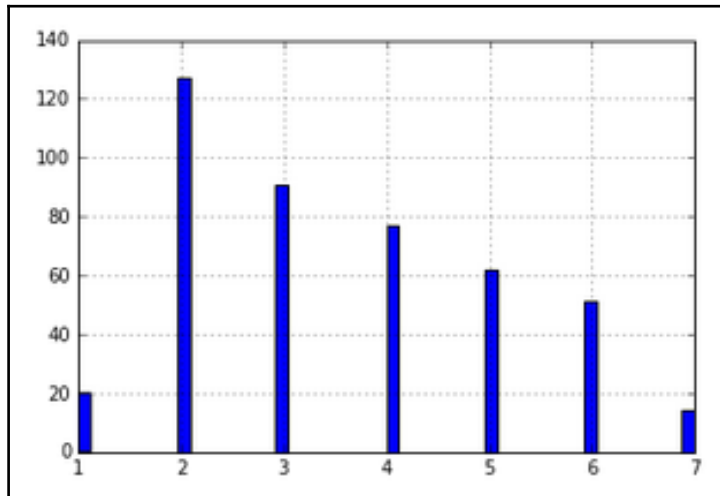
```
bins = 50*np.arange(8)
bins
array([ 0, 50, 100, 150, 200, 250, 300, 350])
```

Using `np.digitize`, bin the target variable:

```
binned_y = np.digitize(y, bins)
```

Visualize the `binned_y` variable with pandas:

```
pd.Series(binned_y).hist(bins=50)
```



The NumPy array `binned_y` keeps track of which bin each element of `y` belongs to. Now, split the set into training and testing sets and stratify the `binned_y` array:

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.2, stratify=binned_y)
```

How to do it...

1. To create a decision tree regressor, instantiate the decision tree and train it:

```
from sklearn.tree import DecisionTreeRegressor

dtr = DecisionTreeRegressor()
dtr.fit(X_train, y_train)
```


2. To measure the model's accuracy, make predictions for the target variable using the test set:

```
y_pred = dtr.predict(X_test)
```

3. Use an error metric to compare `y_test` (ground truth) and `y_pred` (model predictions). Here, use the `mean_absolute_error`, which is the average of the absolute value of the differences between the elements of `y_test` and `y_pred`:

```
from sklearn.metrics import mean_absolute_error
mean_absolute_error(y_test, y_pred)

58.49438202247191
```

4. As an alternative, measure the mean absolute percentage error, which is the average of the absolute value of the differences divided by the size of elements of the ground truth. This measures the magnitude of the error relative to the size of the element of the ground truth:

```
(np.abs(y_test - y_pred) / (y_test)).mean()

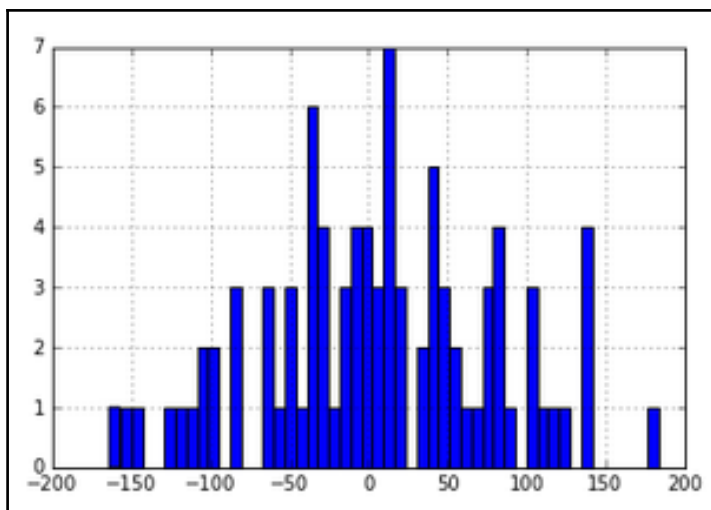
0.4665997687095611
```

Thus, we have established a baseline of performance with regard to the diabetes dataset. Every change to the model will possibly affect the error measurements.

There's more...

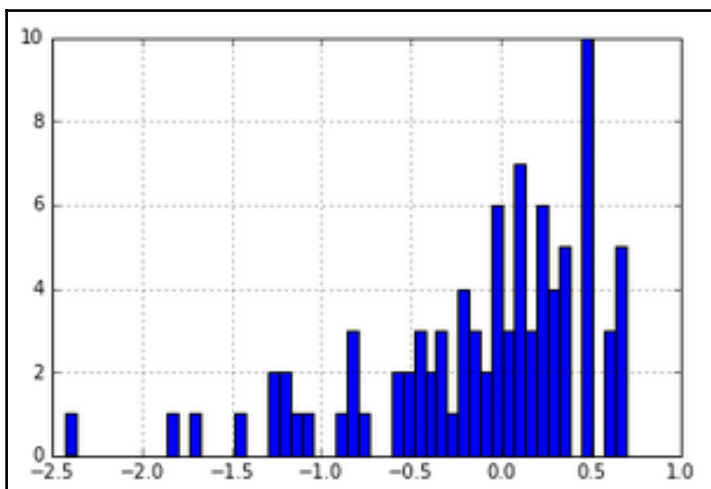
1. With `pandas`, you can quickly visualize the distribution of the errors. Turn the difference between the ground truth, `y_test`, and the predictions, `y_pred`, into a histogram:

```
pd.Series((y_test - y_pred)).hist(bins=50)
```

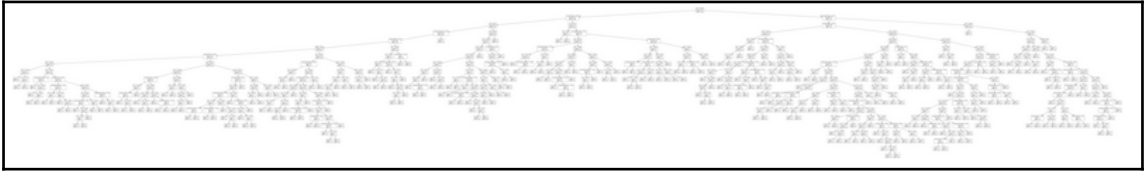


2. You can do the same for the percentage error:

```
pd.Series((y_test - y_pred)/(y_test)).hist(bins=50)
```



3. Finally, using code from previous sections, look at the tree of decisions itself.
Note that we did not optimize for max depth:



The tree is very elaborate and very likely to overfit.

Reducing overfitting with cross-validation

Here, we will use cross-validation on the diabetes dataset from the previous recipe to improve performance. Start by loading the dataset, as in the previous recipe:

```
%matplotlib inline
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import load_diabetes

diabetes = load_diabetes()

X = diabetes.data
y = diabetes.target

X_feature_names = ['age', 'gender', 'body mass index', 'average blood
pressure', 'b1_0', 'b1_1', 'b1_2', 'b1_3', 'b1_4', 'b1_5']

bins = 50*np.arange(8)
binned_y = np.digitize(y, bins)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, stratify=binned_y)
```

How to do it...

1. Use grid search to reduce overfitting. Import a decision tree and instantiate it:

```
from sklearn.tree import DecisionTreeRegressor

dtr = DecisionTreeRegressor()
```

2. Then, import `GridSearchCV` and instantiate this class:

```
from sklearn.model_selection import GridSearchCV

gs_inst = GridSearchCV(dtr, param_grid = {'max_depth':
[3,5,7,9,20]}, cv=10)
gs_inst.fit(X_train, y_train)
```

3. View the best estimator with the `best_estimator_` attribute:

```
gs_inst.best_estimator_

DecisionTreeRegressor(criterion='mse', max_depth=3,
max_features=None,
max_leaf_nodes=None, min_impurity_split=1e-07,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, presort=False, random_state=None,
splitter='best')
```

4. The best estimator has `max_depth` of 3. Now check the error metrics:

```
y_pred = gs_inst.predict(X_test)

from sklearn.metrics import mean_absolute_error
mean_absolute_error(y_test, y_pred)

54.299263338774338
```

5. Check the mean percentage error:

```
(np.abs(y_test - y_pred) / (y_test)).mean()

0.4672742120960478
```

There's more...

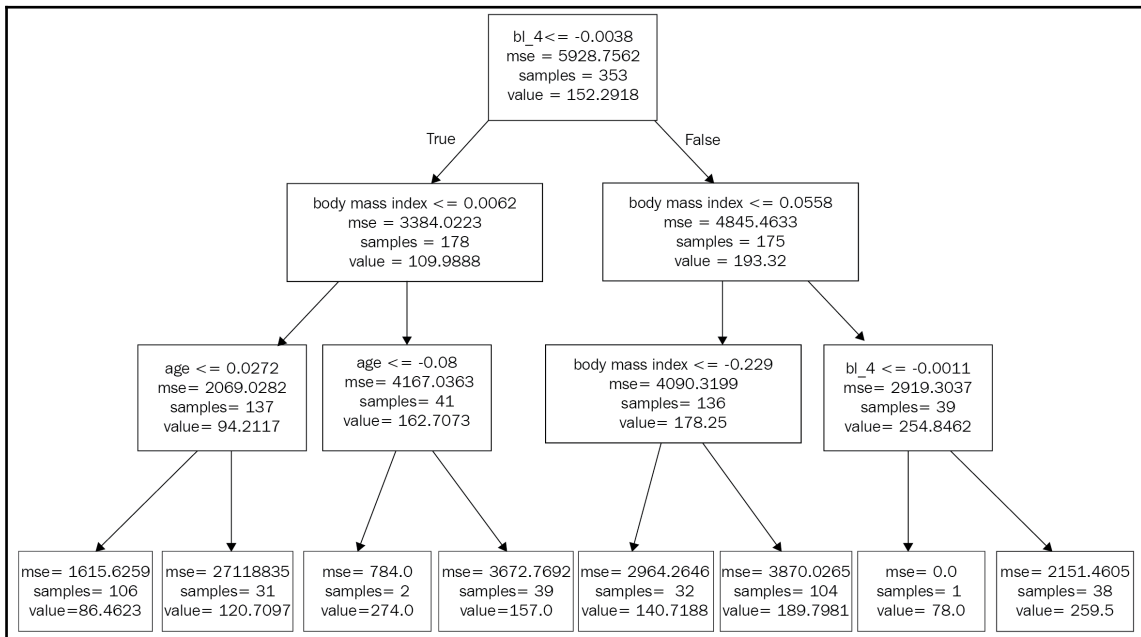
Finally, visualize the best regression tree with graphviz:

```
import numpy as np
from sklearn import tree
from sklearn.externals.six import StringIO

import pydot
from IPython.display import Image

dot_diabetes = StringIO()
tree.export_graphviz(gs_inst.best_estimator_, out_file = dot_diabetes,
feature_names = X_feature_names)
graph = pydot.graph_from_dot_data(dot_diabetes.getvalue())

Image(graph.create_png())
```



The tree has a better accuracy metrics and has been cross-validated to minimize overfitting.

Implementing random forest regression

Random forests is an ensemble algorithm. Ensemble algorithms use several algorithms together to improve predictions. Scikit-learn has several ensemble algorithms, most of which use trees to predict. Let's start by expanding on decision tree regression with several decision trees working together in a random forest.

A random forest is a mixture of several decision trees, where each tree provides a single vote toward the final prediction. The final random forest calculates a final output by averaging the results of all the trees it is composed of.

Getting ready

Load the diabetes regression dataset as we did with decision trees. Split all of the data into training and testing sets:

```
%matplotlib inline

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import load_diabetes

diabetes = load_diabetes()

X = diabetes.data
y = diabetes.target

X_feature_names = ['age', 'gender', 'body mass index', 'average blood
pressure', 'b1_0', 'b1_1', 'b1_2', 'b1_3', 'b1_4', 'b1_5']

#bin target variable for better sampling
bins = 50*np.arange(8)
binned_y = np.digitize(y, bins)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, stratify=binned_y)
```

How to do it...

1. Let's dive in and import and instantiate a random forest. Train the random forest:

```
from sklearn.ensemble import RandomForestRegressor

rft = RandomForestRegressor()
rft.fit(X_train, y_train)
```

2. Measure prediction error. Try the random forest on the test set:

```
y_pred = rft.predict(X_test)

from sklearn.metrics import mean_absolute_error
mean_absolute_error(y_test, y_pred)

48.539325842696627

(np.abs(y_test - y_pred) / (y_test)).mean()

0.42821508503434541
```

The errors have gone down slightly compared to a single decision tree.

3. To access any of the trees that make up the random forest, use the `estimators_` attribute:

```
rft.estimators_

[DecisionTreeRegressor(criterion='mse', max_depth=None,
max_features='auto',
max_leaf_nodes=None, min_impurity_split=1e-07,
min_samples_leaf=1, min_samples_split=2,
min_weight_fraction_leaf=0.0, presort=False,
random_state=492413116, splitter='best')
...]
```

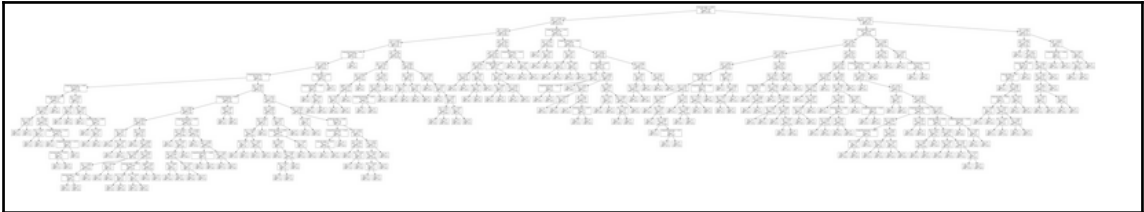
4. To view the first tree on the list in `graphviz`, refer to the first element in the list, `rft.estimators_[0]`:

```
import numpy as np
from sklearn import tree
from sklearn.externals.six import StringIO

import pydot
from IPython.display import Image

dot_diabetes = StringIO()
tree.export_graphviz(rft.estimators_[0], out_file = dot_diabetes,
feature_names = X_feature_names)
graph = pydot.graph_from_dot_data(dot_diabetes.getvalue())

Image(graph.create_png())
```



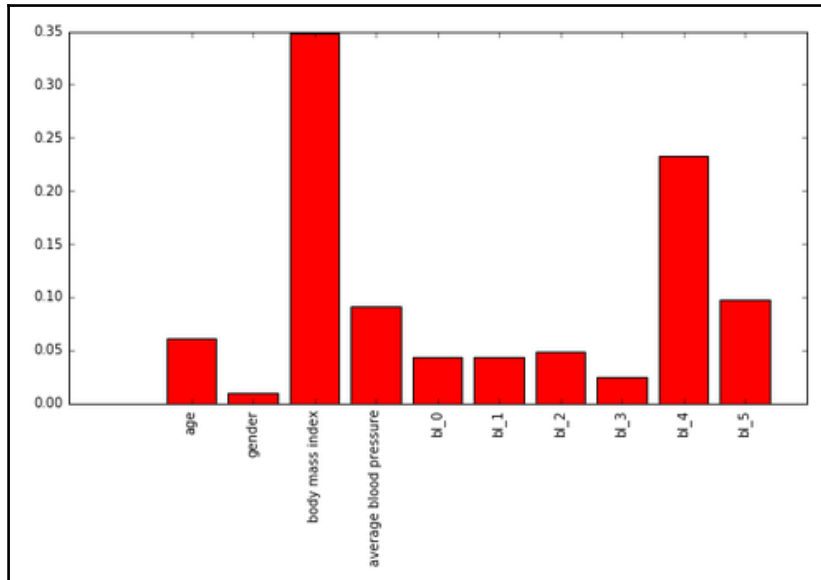
5. To view the second tree, use `best_rft.estimators_[1]`. To view the last tree, use `best_rft.estimators_[9]` because there are, by default, 10 trees, indexed 0 to 9, that make up the random forest.
6. An additional feature of the random forest is determining feature importance through the `feature_importances_` attribute:

```
rft.feature_importances_  
array([ 0.06103037, 0.00969354, 0.34865274, 0.09091215, 0.04331388,  
        0.04376602, 0.04827391, 0.02430837, 0.23251334, 0.09753567])
```


7. You can visualize feature importance as well:

```
fig, ax = plt.subplots(figsize=(10,5))

bar_rects = ax.bar(np.arange(10),
                    rft.feature_importances_, color='r', align='center')
ax.xaxis.set_ticks(np.arange(10))
ax.set_xticklabels(X_feature_names, rotation='vertical')
```



The most influential features are **body mass index (BMI)**, followed by `b1_4` (the fourth of six blood serum measurements), and then average blood pressure.

Bagging regression with nearest neighbors

Bagging is an additional ensemble type that, interestingly, does not necessarily involve trees. It builds several instances of a base estimator acting on random subsets of the first training set. In this section, we try **k-nearest neighbors (KNN)** as the base estimator.

Pragmatically, bagging estimators are great for reducing the variance of a complex base estimator, for example, a decision tree with many levels. On the other hand, boosting reduces the bias of weak models, such as decision trees of very few levels, or linear models.

To try out bagging, we will find the best parameters, a hyperparameter search, using scikit-learn's random grid search. As we have done previously, we will go through the following process:

1. Figure out which parameters to optimize in the algorithm (these are the parameters researchers view as the best to optimize in the literature).
2. Create a parameter distribution where the most important parameters are varied.
3. Perform a random grid search. If you're using an ensemble, keep the number of estimators low at first.
4. Use the best parameters from the previous step with many estimators.

Getting ready

Once more, load the diabetes dataset used in the last section:

```
import numpy as np
import pandas as pd

from sklearn.datasets import load_diabetes
diabetes = load_diabetes()

X = diabetes.data
y = diabetes.target

X_feature_names = ['age', 'gender', 'body mass index', 'average blood
pressure', 'b1_0', 'b1_1', 'b1_2', 'b1_3', 'b1_4', 'b1_5']

#bin target variable for better sampling
bins = 50*np.arange(8)
binned_y = np.digitize(y, bins)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, stratify=binned_y)
```

How to do it...

1. First, import `BaggingRegressor` and `KNeighborsRegressor`. Additionally, also import `RandomizedSearchCV`:

```
from sklearn.ensemble import BaggingRegressor
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import RandomizedSearchCV
```

2. Then, set up a parameter distribution for the grid search. For a bagging meta-estimator, some parameters to vary include `max_samples`, `max_features`, `oob_score`, and the number of estimators, `n_estimators`. The number of estimators is set to a low number, 100, to optimize the other parameters before trying a large number of estimators.
3. Additionally, there is one list of parameters for the KNN algorithm. It is named `base_estimator__n_neighbors`, where `n_neighbors` is the internal name within the KNN class. The `base_estimator` name is the name of the base estimator within the `BaggingRegressor` class. The `base_estimator__n_neighbors` list has the numbers 3 and 5, which refer to the number of neighbors in the nearest neighbors algorithm:

```
param_dist = {
    'max_samples': [0.5, 1.0],
    'max_features' : [0.5, 1.0],
    'oob_score' : [True, False],
    'base_estimator__n_neighbors': [3, 5],
    'n_estimators': [100]
}
```

4. Instantiate the `KNeighborsRegressor` class and pass it as the `base_estimator` within `BaggingRegressor`:

```
single_estimator = KNeighborsRegressor()
ensemble_estimator = BaggingRegressor(base_estimator =
single_estimator)
```

5. Finally, instantiate and run a randomized search. Do a few iterations, `n_iter = 5`, as this could be time consuming:

```
pre_gs_inst_bag = RandomizedSearchCV(ensemble_estimator,
    param_distributions = param_dist,
    cv=3,
    n_iter = 5,
    n_jobs=-1)

pre_gs_inst_bag.fit(X_train, y_train)
```

6. Look at the best parameters in the random search run:

```
pre_gs_inst_bag.best_params_

{'base_estimator__n_neighbors': 5,
 'max_features': 1.0,
 'max_samples': 0.5,
 'n_estimators': 100,
 'oob_score': True}
```

7. Train a `BaggingRegressor` using the best parameters, except for `n_estimators`, which you can increase. We increase the number of estimators to 1,000 in this case:

```
rs_bag = BaggingRegressor(**{'max_features': 1.0,
    'max_samples': 0.5,
    'n_estimators': 1000,
    'oob_score': True,
    'base_estimator': KNeighborsRegressor(n_neighbors=5)})

rs_bag.fit(X_train, y_train)
```

8. Finally, measure the performance on a test set. The algorithm does not perform as well as others, but we can possibly use it as part of a stacking aggregator later:

```
y_pred = rs_bag.predict(X_test)

from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_test, y_pred)
print "MAE : ", mean_absolute_error(y_test, y_pred)
print "MAPE : ", (np.abs(y_test - y_pred) / y_test).mean()

R-squared 0.498096653258
MAE : 44.3642741573
MAPE : 0.419361955306
```

If you look carefully, bagging regression performed slightly better than the random forest in the previous section as both mean absolute error and mean absolute percentage error are better. Always remember that you do not have to limit your ensemble learning to trees—here, you build an ensemble regressor with the KNN algorithm.

Tuning gradient boosting trees

We will examine the California housing dataset with gradient boosting trees. Our overall approach will be the same as before:

1. Focus on important parameters in the gradient boosting algorithm:
 - `max_features`
 - `max_depth`
 - `min_samples_leaf`
 - `learning_rate`
 - `loss`
2. Create a parameter distribution where the most important parameters are varied.
3. Perform a random grid search. If using an ensemble, keep the number of estimators low at first.
4. Use the best parameters from the previous step with many estimators.

Getting ready

Load the California housing dataset and split the loaded dataset into training and testing sets:

```
%matplotlib inline

from __future__ import division #Load within Python 2.7 for regular
division
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import fetch_california_housing

cali_housing = fetch_california_housing()

X = cali_housing.data
y = cali_housing.target
```

```
#bin output variable to split training and testing sets into two similar
sets
bins = np.arange(6)
binned_y = np.digitize(y, bins)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, stratify=binned_y)
```

How to do it...

1. Load the gradient boosting algorithm and random grid search:

```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.model_selection import RandomizedSearchCV
```

2. Create a parameter distribution for the gradient boosting trees:

```
param_dist = {'max_features' : ['log2', 1.0],
              'max_depth' : [3, 5, 7, 10],
              'min_samples_leaf' : [2, 3, 5, 10],
              'n_estimators': [50, 100],
              'learning_rate' : [0.0001, 0.001, 0.01, 0.05, 0.1, 0.3],
              'loss' : ['ls', 'huber']}
}
```

3. Run the grid search to find the best parameters. Perform a randomized search with 30 iterations:

```
pre_gs_inst =
RandomizedSearchCV(GradientBoostingRegressor(warm_start=True),
param_distributions = param_dist,
cv=3,
n_iter = 30, n_jobs=-1)
pre_gs_inst.fit(X_train, y_train)
```

4. Now look at the report in dataframe form. The functions to view the report have been wrapped so that they can be used more times:

```
import numpy as np
import pandas as pd

def get_grid_df(fitted_gs_estimator):
    res_dict = fitted_gs_estimator.cv_results_

    results_df = pd.DataFrame()
    for key in res_dict.keys():
        results_df[key] = res_dict[key]

    return results_df

def group_report(results_df):
    param_cols = [x for x in results_df.columns if 'param' in x
and x is not 'params']
    focus_cols = param_cols + ['mean_test_score']

    print "Grid CV Report \n"

    output_df = pd.DataFrame(columns = ['param_type', 'param_set',
'mean_score', 'mean_std'])
    cc = 0
    for param in param_cols:
        for key, group in results_df.groupby(param):
            output_df.loc[cc] = (param, key,
group['mean_test_score'].mean(), group['mean_test_score'].std())
            cc += 1
    return output_df
```

5. View the dataframe that shows how gradient boosting trees performed with various parameter settings:

```
results_df = get_grid_df(pre_gs_inst)
group_report(results_df)
```

	param_type	param_set	mean_score	mean_std
0	param_loss	huber	0.5741864	0.2992785
1	param_loss	ls	0.6858304	0.1882532
2	param_min_samples_leaf	2	0.605734	0.2303887
3	param_min_samples_leaf	3	0.6768033	0.2124705
4	param_min_samples_leaf	5	0.6758831	0.2509877
5	param_min_samples_leaf	10	0.5858924	0.3397429
6	param_max_depth	3	0.7560831	0.03972102
7	param_max_depth	5	0.6169207	0.3047457
8	param_max_depth	7	0.5333316	0.3141217
9	param_max_depth	10	0.4368587	0.3212123
10	param_learning_rate	0.001	0.0706102	0.03943414
11	param_learning_rate	0.01	0.4928253	0.1112082
12	param_learning_rate	0.05	0.7646034	0.05784881
13	param_learning_rate	0.1	0.7657381	0.02909406
14	param_learning_rate	0.3	0.8003662	0.01720558
15	param_max_features	1	0.6407179	0.2922979
16	param_max_features	log2	0.6190715	0.2433566
17	param_n_estimators	50	0.6115874	0.2344663
18	param_n_estimators	100	0.6391491	0.2801134
19 rows × 4 columns				

From this dataframe; `ls` outperforms `huber` significantly as a loss function, 3 is the best `min_samples_leaf` (but 4 could perform well), 3 is the best `max_depth` (although 1 or 2 could work as well), 0.3 works well as a learning rate (so could 0.2 or 0.4 though), and a `max_features` of 1.0 works well, but so could some other number (such as half of the features: 0.5).

6. With this information, try another randomized search:

```
param_dist = {'max_features' : ['sqrt', 0.5, 1.0],
              'max_depth' : [2, 3, 4],
              'min_samples_leaf' : [3, 4],
              'n_estimators': [50, 100],
```



```

    'learning_rate' : [0.2,0.25, 0.3, 0.4],
    'loss' : ['ls','huber']
}
pre_gs_inst =
RandomizedSearchCV(GradientBoostingRegressor(warm_start=True),
    param_distributions = param_dist,
    cv=3,
    n_iter = 30, n_jobs=-1)
pre_gs_inst.fit(X_train, y_train)

```

7. View the new report that is generated:

```

results_df = get_grid_df(pre_gs_inst)
group_report(results_df)

```

	param_type	param_set	mean_score	mean_std
0	param_loss	huber	0.7931063	0.01673982
1	param_loss	ls	0.7907243	0.02171705
2	param_min_samples_leaf	3	0.7854135	0.02287723
3	param_min_samples_leaf	4	0.7963269	0.01615025
4	param_max_depth	2	0.7670742	0.01904715
5	param_max_depth	3	0.7882193	0.01333549
6	param_max_depth	4	0.805775	0.01076987
7	param_learning_rate	0.2	0.7772841	0.02156672
8	param_learning_rate	0.25	0.79258	0.02690094
9	param_learning_rate	0.3	0.7966627	0.01218264
10	param_learning_rate	0.4	0.7938634	0.01653378
11	param_max_features	0.5	0.8030664	0.01251
12	param_max_features	1	0.7987128	0.01420623
13	param_max_features	sqrt	0.7769333	0.02077015
14	param_n_estimators	50	0.7874801	0.01790079
15	param_n_estimators	100	0.7969823	0.02148434

8. With this information, you can run one more randomized search with the following parameter distributions:

```
param_dist = {'max_features' : [0.4, 0.5, 0.6],
              'max_depth' : [5, 6],
              'min_samples_leaf' : [4, 5],
              'n_estimators': [300],
              'learning_rate' : [0.3],
              'loss' : ['ls', 'huber']}
}
```

9. Storing the result under `rs_gbt`, perform training one last time with 4,000 estimators:

```
rs_gbt = GradientBoostingRegressor(warm_start=True,
                                   max_features = 0.5,
                                   min_samples_leaf = 4,
                                   learning_rate=0.3,
                                   max_depth = 6,
                                   n_estimators = 4000, loss = 'huber')

rs_gbt.fit(X_train, y_train)
```

10. Use scikit-learn's `metrics` module to describe the errors on the test set:

```
y_pred = rs_gbt.predict(X_test)

from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_test, y_pred)
print "MAE : ", mean_absolute_error(y_test, y_pred)
print "MAPE : ", (np.abs(y_test - y_pred) / y_test).mean()

R-squared 0.84490423214
MAE : 0.302125381378
MAPE : 0.169831775387
```

If you recall, the R-squared for the random forest was slightly lower at 0.8252. This algorithm was slightly better. For both, we performed randomized searches. Note that if you perform hyperparameter optimization with trees frequently, you can automate the multiple randomized parameter searches.

There's more...

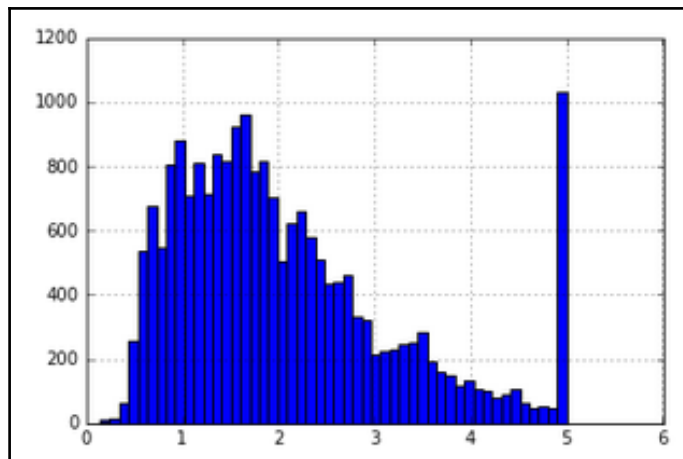
Now, we will optimize a gradient boosting classifier instead of a regressor. The procedure is very similar.

Finding the best parameters of a gradient boosting classifier

Classifying using gradient boosting trees is very similar to the regression we have been doing. Again, we will do the following:

1. Find the best parameters of the gradient boosting classifier. These are the same as the gradient boosting regressor, with the exception that the loss function options are different. The parameters have the same names and are as follows:
 - `max_features`
 - `max_depth`
 - `min_samples_leaf`
 - `learning_rate`
 - `loss`
2. Run an estimator with the best parameter but more trees in the estimator. In the following code, note the change in the loss function called deviance. To do the classification, we will use a binary variable. Recall the visualization of the target set, `y`:

```
pd.Series(y).hist(bins=50)
```



On the far right, there seems to be an anomaly: a lot of values in the distribution are equal to five. Perhaps we would like to separate that set and analyze it separately. As part of that process, we might want to be able to predetermine whether a point should belong to the anomaly set or not. We will build a classifier to separate points where y is equal to or greater than five:

3. First, split the set into training and testing. Stratify the binned variable, `binned_y`:

```
bins = np.arange(6)
binned_y = np.digitize(y, bins)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.2, stratify=binned_y)
```

4. Create a binary variable that has the value 1 if the target variable y is 5 or greater and 0 if it is less than 5. Note that if the binary variable is 1, it belongs to the anomalous set:

```
y_binary = np.where(y >= 5, 1, 0)
```

5. Now, use the shape of `X_train` to split a binary variable into `y_train_binned` and `y_test_binned`:

```
train_shape = X_train.shape[0]

y_train_binned = y_binary[:train_shape]
y_test_binned = y_binary[train_shape:]
```

6. Perform a randomized grid search:

```
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.model_selection import RandomizedSearchCV
param_dist = {'max_features' : ['log2', 0.5, 1.0],
              'max_depth' : [2, 3, 6],
              'min_samples_leaf' : [1, 2, 3, 10],
              'n_estimators' : [100],
              'learning_rate' : [0.1, 0.2, 0.3, 1],
              'loss' : ['deviance']}

pre_gs_inst =
RandomizedSearchCV(GradientBoostingClassifier(warm_start=True),
                  param_distributions = param_dist,
                  cv=3,
                  n_iter = 10, n_jobs=-1)
```

```
pre_gs_inst.fit(X_train, y_train_binned)
```

7. View the best parameters:

```
pre_gs_inst.best_params_  
  
{'learning_rate': 0.2,  
 'loss': 'deviance',  
 'max_depth': 2,  
 'max_features': 1.0,  
 'min_samples_leaf': 2,  
 'n_estimators': 50}
```

8. Increase the number of estimators and train the final estimator:

```
gbc = GradientBoostingClassifier(**{'learning_rate': 0.2,  
 'loss': 'deviance',  
 'max_depth': 2,  
 'max_features': 1.0,  
 'min_samples_leaf': 2,  
 'n_estimators': 1000, 'warm_start': True}).fit(X_train,  
 y_train_binned)
```

9. View the performance of the algorithm:

```
y_pred = gbc.predict(X_test)  
  
from sklearn.metrics import accuracy_score  
accuracy_score(y_test_binned, y_pred)  
  
0.93580426356589153
```

The algorithm, a binary classifier, is about 94% accurate at determining whether the house belongs to the anomalous set. The hyperparameter optimization of the gradient boosting classifier was very similar, with the same important parameters as gradient boosting regression.

Tuning an AdaBoost regressor

The important parameters to vary in an AdaBoost regressor are `learning_rate` and `loss`. As with the previous algorithms, we will perform a randomized parameter search to find the best scores that the algorithm can do.

How to do it...

1. Import the algorithm and randomized grid search. Try a randomized parameter distribution:

```
from sklearn.ensemble import AdaBoostRegressor
from sklearn.model_selection import RandomizedSearchCV

param_dist = {
    'n_estimators': [50, 100],
    'learning_rate' : [0.01, 0.05, 0.1, 0.3, 1],
    'loss' : ['linear', 'square', 'exponential']
}

pre_gs_inst = RandomizedSearchCV(AdaBoostRegressor(),
    param_distributions = param_dist,
    cv=3,
    n_iter = 10,
    n_jobs=-1)

pre_gs_inst.fit(X_train, y_train)
```

2. View the best parameters:

```
pre_gs_inst.best_params_

{'learning_rate': 0.05, 'loss': 'linear', 'n_estimators': 100}
```

3. These suggest another randomized search with parameter distribution:

```
param_dist = {
    'n_estimators': [100],
    'learning_rate' : [0.04, 0.045, 0.05, 0.055, 0.06],
    'loss' : ['linear']
}
```

4. Copy the dictionary that holds the best parameters. Increase the number of estimators in the copy to 3,000:

```
import copy
ada_best = copy.deepcopy(pre_gs_inst.best_params_)
ada_best['n_estimators'] = 3000
```

5. Train the final AdaBoost model:

```
rs_ada = AdaBoostRegressor(**ada_best)
rs_ada.fit(X_train, y_train)
```

6. Measure the model performance on the test set:

```
y_pred = rs_ada.predict(X_test)

from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_test, y_pred)
print "MAE : ", mean_absolute_error(y_test, y_pred)
print "MAPE : ", (np.abs(y_test - y_pred)/y_test).mean()

R-squared 0.485619387823
MAE : 0.708716094846
MAPE : 0.524923208329
```

Unfortunately, this model clearly underperforms relative to the other tree models. We will set it aside without optimizing it any further because it would take more training time and Python development time.

There's more...

We have found the best parameters for a few algorithms. Here is a table summarizing the parameters to optimize for each algorithm under cross-validation. It is suggested you start optimizing these parameters:

Important Variables to Optimize for Various Ensembles/Models	
Decision tree	max_depth
Random forest	max_features, min_samples_leaf, oob_score
Extra trees	max_features, min_samples_leaf, oob_score (same as Random forest)
Bagging ensembles	max_features, max_samples, oob_score, any parameters of the base estimators
Gradient boosting trees	max_features, max_depth, min_samples_leaf, learning_rate, loss
Ada boost	learning_rate, loss, any parameters of the base estimators

Writing a stacking aggregator with scikit-learn

In this section, we will write a stacking aggregator with scikit-learn. A stacking aggregator mixes models of potentially very different types. Many of the ensemble algorithms we have seen mix models of the same type, usually decision trees.

The fundamental process in the stacking aggregator is that we use the predictions of several machine learning algorithms as input for the training of another machine learning algorithm.

In more detail, we train two or more machine learning algorithms using a pair of X and y sets (X_1 , y_1). Then we make predictions on a second X set (X_{stack}), y_{pred_1} , y_{pred_2} , and so on.

These predictions, y_{pred_1} and y_{pred_2} , become inputs to a machine learning algorithm with the training output y_{stack} . Finally, the error can be measured on a third input set, X_3 , and a ground truth set, y_3 .

It will be easier to see in an example.

How to do it...

1. Load the data from the California housing dataset once again. Observe how we create bins once more to stratify a continuous variable:

```
%matplotlib inline

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import fetch_california_housing

cali_housing = fetch_california_housing()

X = cali_housing.data
y = cali_housing.target

bins = np.arange(6)

from __future__ import division
```



```

from sklearn.model_selection import train_test_split

binned_y = np.digitize(y, bins)

from sklearn.ensemble import RandomForestRegressor,
AdaBoostRegressor, ExtraTreesRegressor, GradientBoostingRegressor

from sklearn.model_selection import GridSearchCV

```

2. Now split the pair, x and y , into three x and y pairs, input and output, by using `train_test_split` twice. Note how we stratify the continuous variable at each stage:

```

X_train_prin, X_test_prin, y_train_prin, y_test_prin =
train_test_split(X, y,
    test_size=0.2,
    stratify=binned_y)

binned_y_train_prin = np.digitize(y_train_prin, bins)

X_1, X_stack, y_1, y_stack = train_test_split(X_train_prin,
    y_train_prin,
    test_size=0.33,
    stratify=binned_y_train_prin )

```

3. Using `RandomizedSearchCV`, find the best parameters for the first of the algorithms in the stacking aggregator, in this case a bagging algorithm of several nearest neighbor models:

```

from sklearn.ensemble import BaggingRegressor
from sklearn.neighbors import KNeighborsRegressor

from sklearn.model_selection import RandomizedSearchCV

param_dist = {
    'max_samples': [0.5,1.0],
    'max_features' : [0.5,1.0],
    'oob_score' : [True, False],
    'base_estimator__n_neighbors': [3,5],
    'n_estimators': [100]
}

single_estimator = KNeighborsRegressor()
ensemble_estimator = BaggingRegressor(base_estimator =
single_estimator)

pre_gs_inst_bag = RandomizedSearchCV(ensemble_estimator,

```

```
param_distributions = param_dist,
cv=3,
n_iter = 5,
n_jobs=-1)
```

```
pre_gs_inst_bag.fit(X_1, y_1)
```

4. Using the best parameters, train the bagging regressor using many estimators, in this case, 3,000:

```
rs_bag = BaggingRegressor(**{'max_features': 0.5,
    'max_samples': 0.5,
    'n_estimators': 3000,
    'oob_score': False,
    'base_estimator': KNeighborsRegressor(n_neighbors=3)})
```

```
rs_bag.fit(X_1, y_1)
```

5. Do the same process for the gradient boost algorithm on the X_1, y_1 pair of sets:

```
from sklearn.ensemble import GradientBoostingRegressor
from sklearn.model_selection import RandomizedSearchCV

param_dist = {'max_features' : ['log2', 0.4, 0.5, 0.6, 1.0],
    'max_depth' : [2, 3, 4, 5, 6, 7, 10],
    'min_samples_leaf' : [1, 2, 3, 4, 5, 10],
    'n_estimators' : [50, 100],
    'learning_rate' : [0.01, 0.05, 0.1, 0.25, 0.275, 0.3, 0.325],
    'loss' : ['ls', 'huber']
}
pre_gs_inst =
RandomizedSearchCV(GradientBoostingRegressor(warm_start=True),
param_distributions = param_dist,
cv=3,
n_iter = 30, n_jobs=-1)
pre_gs_inst.fit(X_1, y_1)
```

6. Train the best parameter set with more estimators:

```
gbt_inst = GradientBoostingRegressor(**{'learning_rate': 0.05,
    'loss': 'huber',
    'max_depth': 10,
    'max_features': 0.4,
    'min_samples_leaf': 5,
    'n_estimators': 3000,
    'warm_start': True}).fit(X_1, y_1)
```

7. Predict the target using `X_stack` using both algorithms:

```
y_pred_bag = rs_bag.predict(X_stack)
y_pred_gbt = gbt_inst.predict(X_stack)
```

8. View the metrics (error rates) that each algorithm produces. View the metrics for the bagging regressor:

```
from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_stack, y_pred_bag)
print "MAE : ", mean_absolute_error(y_stack, y_pred_bag)
print "MAPE : ", (np.abs(y_stack - y_pred_bag) / y_stack).mean()

R-squared 0.527045729567
MAE : 0.605868386902
MAPE : 0.397345752723
```

9. View the metrics for gradient boost:

```
from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_stack, y_pred_gbt)
print "MAE : ", mean_absolute_error(y_stack, y_pred_gbt)
print "MAPE : ", (np.abs(y_stack - y_pred_gbt) / y_stack).mean()

R-squared 0.841011059404
MAE : 0.297099247278
MAPE : 0.163956322255
```

10. Create a dataframe of the predictions from both algorithms. Alternatively, you could also create a NumPy array of the data:

```
y_pred_bag = rs_bag.predict(X_stack)
y_pred_gbt = gbt_inst.predict(X_stack)

preds_df = pd.DataFrame(columns = ['bag', 'gbt'])

preds_df['bag'] = y_pred_bag
preds_df['gbt'] = y_pred_gbt
```

11. View the new dataframe of predictions:

```
preds_df
```

	bag	gbt
0	1.719959	1.259770
1	2.057504	2.630964
2	2.443155	3.392195
3	2.305488	2.849641
4	1.753468	1.419086
5	2.302396	3.761979
6	2.217249	3.648032
7	1.282082	0.654588

12. Look at the correlation between the prediction columns. The columns are correlated, but not perfectly. The ideal situation is that the algorithms are not perfectly correlated and both perform well. In this case, the bagging regressor does not perform nearly as well as gradient boost:

```
preds_df.corr()
```

	bag	gbt
bag	1.000000	0.904855
gbt	0.904855	1.000000

13. Now do a randomized search with a third algorithm. This algorithm takes as input the predictions of the first two. We will use an extra trees regressor to make predictions on the predictions of the other two algorithms:

```
from sklearn.ensemble import ExtraTreesRegressor
from sklearn.model_selection import RandomizedSearchCV

param_dist = {'max_features' : ['sqrt', 'log2', 1.0],
              'min_samples_leaf' : [1, 2, 3, 7, 11],
              'n_estimators': [50, 100],
```

```

    'oob_score': [True, False]}

pre_gs_inst =
RandomizedSearchCV(ExtraTreesRegressor(warm_start=True, bootstrap=True),
    param_distributions = param_dist,
    cv=3,
    n_iter = 15)

pre_gs_inst.fit(preds_df.values, y_stack)

```

14. Copy the parameter dictionary and increase the number of estimators within that copied dictionary. View the final dictionary, if you want to:

```

import copy

param_dict = copy.deepcopy(pre_gs_inst.best_params_)

param_dict['n_estimators'] = 2000
param_dict['warm_start'] = True
param_dict['bootstrap'] = True
param_dict['n_jobs'] = -1

param_dict

{'bootstrap': True,
 'max_features': 1.0,
 'min_samples_leaf': 11,
 'n_estimators': 2000,
 'n_jobs': -1,
 'oob_score': False,
 'warm_start': True}

```

15. Train the extra trees regressor on the predictions dataframe using `y_stack` as a target:

```

final_etr = ExtraTreesRegressor(**param_dict)
final_etr.fit(preds_df.values, y_stack)

```

16. To examine the overall performance of the stacking aggregator, you need a function that takes an `x` set as input, predicts creating a dataframe using the bagging regressor and gradient boost, and finally predicts on those predictions:

```

def handle_X_set(X_train_set):
    y_pred_bag = rs_bag.predict(X_train_set)
    y_pred_gbt = gbt_inst.predict(X_train_set)
    preds_df = pd.DataFrame(columns = ['bag', 'gbt'])

```

```

    preds_df['bag'] = y_pred_bag
    preds_df['gbt'] = y_pred_gbt

    return preds_df.values

def predict_from_X_set(X_train_set):
    return final_etr.predict(handle_X_set(X_train_set))

```

17. Predict using `X_test_prin`, the X set that was left out, using the useful `predict_from_X_set` function we just created:

```
y_pred = predict_from_X_set(X_test_prin)
```

18. Measure the performance of the model:

```

from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_test_prin, y_pred)
print "MAE : ", mean_absolute_error(y_test_prin, y_pred)
print "MAPE : ", (np.abs(y_test_prin - y_pred) / y_test_prin).mean()

R-squared 0.844114615094
MAE : 0.298422222752
MAPE : 0.173901911714

```

What now? The R-squared metric improved slightly, and we worked very hard for that slight improvement. What we could do next is write more robust, production-like code for the stacker that makes it easy to place a lot of estimators that are not correlated within the stacker.

Additionally, we could do feature engineering—improving the columns of the data using math and/or domain knowledge of the California housing industry. You can also try different algorithms for different inputs. Two columns, latitude and longitude, are well suited for random forests and other inputs could be well-modeled with a linear algorithm.

Thirdly, we could explore different algorithms on the dataset. For this dataset we focused on complex, high-variance algorithms. We could try simpler high-bias algorithms. These alternative algorithms could help the stacking aggregator we used at the end.

Finally, in regards to the stacker, you could rotate the `X_stacker` set through cross-validation to make the most of the training set.

10

Text and Multiclass Classification with scikit-learn

This chapter will cover the following recipes:

- Using LDA for classification
- Working with QDA – a nonlinear LDA
- Using SGD for classification
- Classifying documents with Naive Bayes
- Label propagation with semi-supervised learning

Using LDA for classification

Linear discriminant analysis (LDA) attempts to fit a linear combination of features to predict an outcome variable. LDA is often used as a pre-processing step. We'll walk through both methods in this recipe.

Getting ready

In this recipe, we will do the following:

1. Grab stock data from Google.
2. Rearrange it in a shape we're comfortable with.
3. Create an LDA object to fit and predict the class labels.
4. Give an example of how to use LDA for dimensionality reduction.

Before starting on step 1 and grabbing stock data from Google, install a version of pandas that supports the latest stock reader. Do so at an Anaconda command line by typing this:

```
conda install -c anaconda pandas-datareader
```

Note that your pandas version will be updated. If this is a problem, create a new environment for this pandas version. Now open a notebook and check whether the pandas-datareader imports correctly:

```
from pandas-datareader import data
```

If it is imported correctly, no errors will show up.

How to do it...

In this example, we will perform an analysis similar to Altman's Z-score. In his paper, Altman looked at a company's likelihood of defaulting within two years based on several financial metrics. The following is taken from the Wikipedia page of Altman's Z-score:

Z-score formula	Description
$T1 = \text{Working capital} / \text{Total assets}$	This measures liquid assets in relation to the size of the company.
$T2 = \text{Retained earnings} / \text{Total assets}$	This measures profitability that reflects the company's age and earning power.
$T3 = \text{Earnings before interest and taxes} / \text{Total assets}$	This measures operating efficiency apart from tax and leveraging factors. It recognizes operating earnings as being important to long-term viability.
$T4 = \text{Market value of equity} / \text{Book value of total liabilities}$	This adds market dimension that can show up a security price fluctuation as a possible red flag.
$T5 = \text{Sales} / \text{Total assets}$	This is the standard measure for total asset turnover (varies greatly from industry to industry).

Refer to the article, *Financial Ratios, Discriminant Analysis and the Prediction of Corporate Bankruptcy*, by Altman, Edward I. (September 1968), *Journal of Finance*: 189–209.

In this analysis, we'll look at some financial data from Google via pandas. We'll try to predict whether a stock will be higher in exactly six months from today based on the current attribute of the stock. It's obviously nowhere near as refined as Altman's Z-score.

1. Begin with a few imports and by storing the tickers you will use, the first date, and the last date of the data:

```
%matplotlib inline

from pandas_datareader import data
import pandas as pd

tickers = ["F", "TM", "GM", "TSLA"]

first_date = '2009-01-01'
last_date = '2016-12-31'
```

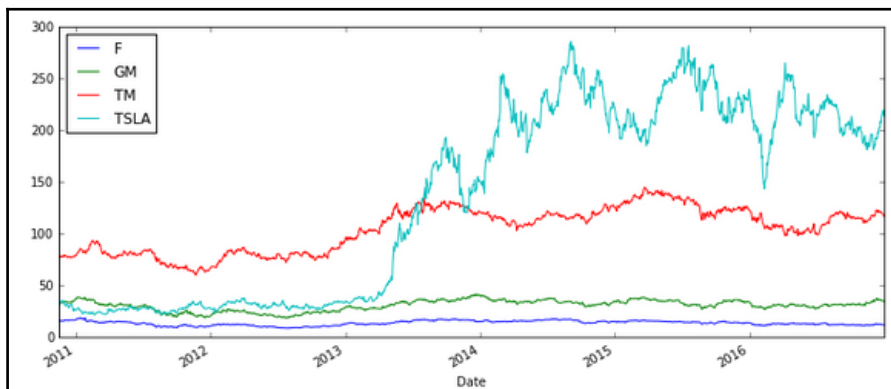
2. Now, let's pull the stock data:

```
stock_panel = data.DataReader(tickers, 'google', first_date,
                               last_date)
```

3. This data structure is a panel from pandas. It's similar to an **online analytical processing (OLAP)** cube or a 3D dataframe. Let's take a look at the data to get more familiar with the closes since that's what we care about when comparing:

```
stock_df = stock_panel.Close.dropna()
stock_df.plot(figsize=(12, 5))
```

The following is the output:



Okay, so now we need to compare each stock price with its price in six months. If it's higher, we'll code it with one, and if not, we'll code it with zero.

4. To do this, we'll just shift the dataframe back by 180 days and compare:

```
#this dataframe indicates if the stock was higher in 180 days
classes = (stock_df.shift(-180) > stock_df).astype(int)
```

5. The next thing we need to do is flatten out the dataset:

```
X = stock_panel.to_frame()
classes = classes.unstack()
classes = classes.swaplevel(0, 1).sort_index()
classes = classes.to_frame()
classes.index.names = ['Date', 'minor']
data = X.join(classes).dropna()
data.rename(columns={0: 'is_higher'}, inplace=True)
data.head()
```

The following is the output:

		Open	High	Low	Close	Volume	is_higher
Date	minor						
2010-11-18	F	16.77	16.87	16.05	16.12	256937875.0	0.0
	GM	35.00	35.99	33.89	34.19	458097672.0	0.0
	TM	77.36	77.51	76.83	77.29	992235.0	0.0
	TSLA	30.67	30.74	28.92	29.89	956248.0	0.0
2010-11-19	F	16.02	16.38	15.83	16.28	130323560.0	0.0

6. Okay, so now we need to create matrices in NumPy. To do this, we'll use the `patsy` library. This is a great library that can be used to create a design matrix in a fashion similar to R:

```
import patsy
X = patsy.dmatrix("Open + High + Low + Close + Volume + is_higher - 1", data.reset_index(), return_type='dataframe')
X.head()
```

The following is the output:

	Open	High	Low	Close	Volume	is_higher
0	16.77	16.87	16.05	16.12	256937875.0	0.0
1	35.00	35.99	33.89	34.19	458097672.0	0.0
2	77.36	77.51	76.83	77.29	992235.0	0.0
3	30.67	30.74	28.92	29.89	956248.0	0.0
4	16.02	16.38	15.83	16.28	130323560.0	0.0

The `patsy` is a very strong package; for example, suppose we want to apply pre-processing. In `patsy`, it's possible, like R, to modify the formula in a way that corresponds to modifications in the design matrix. It won't be done here, but if we want to scale the value to mean 0 and standard deviation 1, the function will be `scale(open) + scale(high)`.

7. So, now that we have our dataset, let's fit the LDA object:

```
from sklearn.discriminant_analysis import
LinearDiscriminantAnalysis as LDA
lda = LDA()
lda.fit(X.iloc[:, :-1], X.iloc[:, -1]);
```

8. We can see that it's not too bad when predicting against the dataset. Certainly, we will want to improve this with other parameters and test the model:

```
from sklearn.metrics import classification_report
print classification_report(X.iloc[:, -1].values,
lda.predict(X.iloc[:, :-1]))
```

	precision	recall	f1-score	support
0.0	0.64	0.81	0.72	3432
1.0	0.64	0.42	0.51	2727
avg / total	0.64	0.64	0.62	6159

These metrics describe how the model fits the data in various ways.

The `precision` and `recall` parameters are fairly similar. In some ways, as shown in the following list, they can be thought of as conditional proportions:

- `precision`: Given that the model predicts a positive value, what proportion of it is correct? This is why an alternate name for precision is **positive predictive value (PPV)**.
- `recall`: Given that the state of one class is true, what proportion did we select? I say select because `recall` is a common metric in search problems. For example, there can be a set of underlying web pages that, in fact, relate to a search term—the proportion that is returned. In [Chapter 5, Linear Models - Logistic Regression](#), you saw `recall` by another name, sensitivity.

The `f1-score` parameter attempts to summarize the relationship between `recall` and `precision`.

How it works...

LDA is actually fairly similar to clustering, which we did previously. We fit a basic model from the data. Then, once we have the model, we try to predict and compare the likelihoods of the data given in each class. We choose the option that is more likely.

LDA is actually a simplification of **quadratic discernment analysis (QDA)**, which we'll talk about in the next recipe. Here we assume that the covariance of each class is the same, but in QDA, this assumption is relaxed. Think about the connections between KNN and **Gaussian mixture models (GMM)** and the relationship there and here.

Working with QDA – a nonlinear LDA

QDA is the generalization of a common technique such as quadratic regression. It is simply a generalization of a model to allow for more complex models to fit, though, like all things, when allowing complexity to creep in, we make our lives more difficult.

Getting ready

We will expand on the last recipe and look at QDA via the QDA object.

We said we made an assumption about the covariance of the model. Here we will relax that assumption.

How to do it...

1. QDA is aptly a member of the `qda` module. Use the following commands to use QDA:

```
from sklearn.discriminant_analysis import
QuadraticDiscriminantAnalysis as QDA
qda = QDA()

qda.fit(X.iloc[:, :-1], X.iloc[:, -1])
predictions = qda.predict(X.iloc[:, :-1])
predictions.sum()

2686.0

from sklearn.metrics import classification_report
print classification_report(X.iloc[:, -1].values, predictions)
           precision    recall  f1-score   support

    0.0           0.65       0.66       0.65         3432
    1.0           0.56       0.55       0.56         2727

 avg / total           0.61       0.61       0.61        6159
```

As you can see, it's about equal on the whole. If we look back at the *Using LDA for classification* recipe, we can see large changes as opposed to the QDA object for class zero and minor differences for class one.

As we talked about in the last recipe, we essentially compare likelihoods here. But how do we compare likelihoods? Let's just use the price at hand to attempt to classify `is_higher`.

How it works...

We'll assume that the closing price is log-normally distributed. In order to compute the likelihood for each class, we need to create the subsets of the closes as well as a training and test set for each class. We'll use the built-in cross-validation methods:

```
from sklearn.model_selection import ShuffleSplit
import scipy.stats as sp

shuffle_split_inst = ShuffleSplit()

for test, train in shuffle_split_inst.split(X):
    train_set = X.iloc[train]
    train_close = train_set.Close
```

```
train_0 = train_close[~train_set.is_higher.astype(bool)]
train_1 = train_close[train_set.is_higher.astype(bool)]

test_set = X.iloc[test]
test_close = test_set.Close.values

ll_0 = sp.norm.pdf(test_close, train_0.mean())
ll_1 = sp.norm.pdf(test_close, train_1.mean())
```

Now that we have likelihoods for both classes, we can compare and assign classes:

```
(ll_0 > ll_1).mean()

0.14486740032473389
```

Using SGD for classification

The **stochastic gradient descent** (SGD) is a fundamental technique used to fit a model for regression. There are natural connections between SGD for classification or regression.

Getting ready

In regression, we minimized a cost function that penalized for bad choices on a continuous scale, but for classification, we'll minimize a cost function that penalizes for two (or more) cases.

How to do it...

1. First, let's create some very basic data:

```
from sklearn import datasets
X, y = datasets.make_classification(n_samples = 500)
```

2. Split the data into training and testing sets:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y)
```

3. Instantiate and train the classifier:

```
from sklearn import linear_model
sgd_clf = linear_model.SGDClassifier()
#As usual, we'll fit the model:
sgd_clf.fit(X_train, y_train)
```

4. Measure the performance on the test set:

```
from sklearn.metrics import accuracy_score
accuracy_score(y_test, sgd_clf.predict(X_test))

0.80000000000000004
```

There's more...

We can set the `class_weight` parameter to account for the varying amount of imbalance in a dataset.

The hinge loss function is defined as follows:

$$\max(0, 1 - ty)$$

Here, t is the true classification denoted as $+1$ for one case and -1 for the other. The vector of coefficients is denoted by y as fit from the model, and x is the value of interest. There is also an intercept for good measure. To put it another way:

$$t \in -1, 1$$

$$y = \beta x + b$$

Classifying documents with Naive Bayes

Naive Bayes is a really interesting model. It's somewhat similar to KNN in the sense that it makes some assumptions that might oversimplify reality, but still it performs well in many cases.

Getting ready

In this recipe, we'll use Naive Bayes to do document classification with `sklearn`. An example I have personal experience of is using a word that makes up an account descriptor in accounting, such as accounts payable, and determining if it belongs to the income statement, cash flow statement, or balance sheet.

The basic idea is to use the word frequency from a labeled test corpus to learn the classifications of the documents. Then, we can turn it on a training set and attempt to predict the label.

We'll use the `newsgroups` dataset within `sklearn` to play with the Naive Bayes model. It's a non-trivial amount of data, so we'll fetch it instead of loading it. We'll also limit the categories to `rec.autos` and `rec.motorcycles`:

```
import numpy as np
from sklearn.datasets import fetch_20newsgroups
categories = ["rec.autos", "rec.motorcycles"]
newsgroups = fetch_20newsgroups(categories=categories)
#take a look
print "\n".join(newsgroups.data[:1])

From: greg1@zimmer.CSUFresno.EDU (Greg Lewis)
Subject: Re: WARNING.....(please read)...
Keywords: BRICK, TRUCK, DANGER
Nntp-Posting-Host: zimmer.csufresno.edu
Organization: CSU Fresno
Lines: 33
...

newsgroups.target_names

['rec.autos', 'rec.motorcycles']
```

Now that we have new groups, we'll need to represent each document as a bag-of-words. This representation is what gives Naive Bayes its name. The model is naive because documents are classified without regard for any intradocument word covariance. This might be considered a flaw, but Naive Bayes has been shown to work reasonably well.

We need to pre-process the data into a bag-of-words matrix. This is a sparse matrix that has entries when the word is present in the document. This matrix can become quite large, as illustrated:

```
from sklearn.feature_extraction.text import CountVectorizer
count_vec = CountVectorizer()
bow = count_vec.fit_transform(newgroups.data)
```

This matrix is a sparse matrix, which is the length of the number of documents by each word. The document and word value of the matrix are the frequency of the particular term:

```
bow

<1192x19177 sparse matrix of type '<type 'numpy.int64'>'
with 164296 stored elements in Compressed Sparse Row format>
```

We'll actually need the matrix as a dense array for the Naive Bayes object. So, let's convert it back:

```
bow = np.array(bow.todense())
```

Clearly, most of the entries are zero, but we might want to reconstruct the document counts as a sanity check:

```
words = np.array(count_vec.get_feature_names())
words[bow[0] > 0][:5]

array([u'10pm', u'1qh336innf15', u'33', u'93740',
       u'_____'],
      dtype='<U79')
```

Now, are these the examples in the first document? Let's check that using the following command:

```
'10pm' in newgroups.data[0].lower()

True

'1qh336innf15' in newgroups.data[0].lower()

True
```

How to do it...

Okay, so it took a bit longer than normal to get the data ready, but we're dealing with text data that isn't as quickly represented as a matrix as the data we're used to.

1. However, now that we're ready, we'll fire up the classifier and fit our model:

```
from sklearn import naive_bayes
clf = naive_bayes.GaussianNB().fit(X_train, y_train)
```

2. Rename the sets `bow` and `newgroups.target` to `X` and `y` respectively. Before we fit the model, let's split the dataset into a training and a test set:

```
X = bow
y = newgroups.target

from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size
= 0.5, stratify=y)
```

3. Now that we fit a model on a test set and predicted the training set in an attempt to determine which categories go with which articles, let's get a sense of the approximate accuracy:

```
from sklearn.metrics import accuracy_score
accuracy_score(y_test, clf.predict(X_test) )

0.94630872483221473
```

How it works...

The fundamental idea of Naive Bayes is that we can estimate the probability of a data point being a class, given the feature vector.

This can be rearranged via the Bayes formula to give the **maximum a posteriori (MAP)** estimate for the feature vector. This MAP estimate chooses the class for which the feature vector's probability is maximized.

There's more...

We can also extend Naive Bayes to do multiclass work. Instead of assuming a Gaussian likelihood, we'll use a multinomial likelihood.

First, let's get a third category of data:

```
from sklearn.datasets import fetch_20newsgroups
mn_categories = ["rec.autos", "rec.motorcycles", "talk.politics.guns"]
mn_newgroups = fetch_20newsgroups(categories=mn_categories)
```

We'll need to vectorize this just like the class case:

```
mn_bow = count_vec.fit_transform(mn_newgroups.data)
mn_bow = np.array(mn_bow.todense())
```

Rename `mn_bow` and `mn_newgroups.target` to `X` and `y` respectively. Let's create a train and a test set and train a multinomial Bayes model with the training data:

```
X = mn_bow
y = mn_newgroups.target

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size =
0.5, stratify=y)

from sklearn.naive_bayes import MultinomialNB
clf = MultinomialNB().fit(X_train, y_train)
```

Measure the model accuracy:

```
from sklearn.metrics import accuracy_score
accuracy_score(y_test, clf.predict(X_test))

0.96317606444188719
```

It's not completely surprising that we did well. We did fairly well in the dual class case, and since one will guess that the `talk.politics.guns` category is fairly orthogonal to the other two, we should probably do pretty well.

Label propagation with semi-supervised learning

Label propagation is a semi-supervised technique that makes use of labeled and unlabeled data to learn about unlabeled data. Quite often, data that will benefit from a classification algorithm is difficult to label. For example, labeling data might be very expensive, so only a subset is cost-effective to manually label. That said, there does seem to be slow but growing support for companies to hire taxonomists.

Getting ready

Another problem area is censored data. You can imagine a case where the frontier of time will affect your ability to gather labeled data. Say, for instance, you took measurements of patients and gave them an experimental drug. In some cases, you are able to measure the outcome of the drug if it happens fast enough, but you might want to predict the outcome of the drugs that have a slower reaction time. The drug might cause a fatal reaction for some patients and life-saving measures might need to be taken.

How to do it...

1. In order to represent semi-supervised or censored data, we'll need to do a little data pre-processing. First, we'll walk through a simple example, and then we'll move on to some more difficult cases:

```
from sklearn import datasets
d = datasets.load_iris()
```

2. Due to the fact that we'll be messing with the data, let's make copies and add an unlabeled member to the target name's copy. It'll make it easier to identify the data later:

```
x = d.data.copy()
y = d.target.copy()
names = d.target_names.copy()
names = np.append(names, ['unlabeled'])
names

array(['setosa', 'versicolor', 'virginica', 'unlabeled'],
      dtype='<S10')
```

3. Now, let's update `y` with `-1`. This is the marker for the unlabeled case. This is also why we added unlabeled at the end of the names:

```
y[np.random.choice([True, False], len(y))] = -1
```

4. Our data now has a bunch of negative ones (`-1`) interspersed with the actual data:

```
y[:10]

array([ 0, -1, -1, 0, 0, 0, 0, -1, 0, -1])

names[y[:10]]

array(['setosa', 'unlabeled', 'unlabeled', 'setosa', 'setosa',
      'setosa',
      'setosa', 'unlabeled', 'setosa', 'unlabeled'],
      dtype='<S10')
```

5. We clearly have a lot of unlabeled data, and the goal now is to use the `LabelPropagation` method to predict the labels:

```
from sklearn import semi_supervised
lp = semi_supervised.LabelPropagation()
lp.fit(X, y)

LabelPropagation(alpha=1, gamma=20, kernel='rbf', max_iter=30,
n_jobs=1,
n_neighbors=7, tol=0.001)
```

6. Measure the accuracy score:

```
preds = lp.predict(X)
(preds == d.target).mean()

0.9733333333333333
```

Not too bad, though we did use all the data, so it's kind of cheating. Also, the iris dataset is a fairly separated dataset.



Using the whole dataset is reminiscent of more traditional statistics. Making the choice of not measuring on a test set decreases our focus on prediction and encourages more understanding and interpretation of the whole dataset. As mentioned before, understanding versus black-box prediction distinguishes traditional statistics with machine learning.

While we're at it, let's look at `LabelSpreading`, the sister class of `LabelPropagation`. We'll make the technical distinction between `LabelPropagation` and `LabelSpreading` in the *How it works...* section of this recipe, but they are extremely similar:

```
ls = semi_supervised.LabelSpreading()
```

The `LabelSpreading` is more robust and noisy as observed from the way it works:

```
ls.fit(X, y)

LabelSpreading(alpha=0.2, gamma=20, kernel='rbf', max_iter=30, n_jobs=1,
               n_neighbors=7, tol=0.001)
```

Measure the accuracy score:

```
(ls.predict(X) == d.target).mean()

0.9666666666666667
```

Don't consider the fact that the label-spreading algorithm missed one more as an indication and that it performs worse in general. The whole point is that we might give it some ability to predict well on the training set and to work on a wider range of situations.

How it works...

Label propagation works by creating a graph of the data points, with weights placed on the edge as per the following formula:

$$w_{ij}(\theta) = \frac{d_{ij}}{\theta^2}$$

The algorithm then works by labeled data points propagating their labels to the unlabeled data. This propagation is, in part, determined by edge weight.

The edge weights can be placed in a matrix of transition probabilities. We can iteratively determine a good estimate of the actual labels.

11

Neural Networks

In this chapter we will cover the following recipes:

- Perceptron classifier
- Neural network – multilayer perceptron
- Stacking with a neural network

Introduction

Neural networks and deep learning have been incredibly popular recently as they have solved tough problems and perhaps have become a significant part of the public face of artificial intelligence. Let's explore the feed-forward neural networks available in scikit-learn.

Perceptron classifier

With scikit-learn, you can explore the perceptron classifier and relate it to other classification procedures within scikit-learn. Additionally, perceptrons are the building blocks of neural networks, which are a very prominent part of machine learning, particularly computer vision.

Getting ready

Let's get started. The process is as follows:

1. Load the UCI diabetes classification dataset.
2. Split the dataset into training and test sets.
3. Import a perceptron.
4. Instantiate the perceptron.
5. Then train the perceptron.
6. Try the perceptron on the testing set or preferably compute `cross_val_score`.

Load the UCI diabetes dataset:

```
import numpy as np
import pandas as pd

data_web_address =
"https://archive.ics.uci.edu/ml/machine-learning-databases/pima-indians-diabetes/pima-indians-diabetes.data"

column_names = ['pregnancy_x',
'plasma_con',
'blood_pressure',
'skin_mm',
'insulin',
'bmi',
'pedigree_func',
'age',
'target']

feature_names = column_names[:-1]

all_data = pd.read_csv(data_web_address , names=column_names)

X = all_data[feature_names]
y = all_data['target']
```

You have loaded `x`, the set of input features, and `y`, the variable we desired to predict. Split `x` and `y` into testing and training sets. Do this by stratifying the target set, keeping the classes in balanced proportions in both training and testing sets:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, stratify=y)
```


How to do it...

1. Scale the set of features. Perform the scaling operation on the training set only and then continue with the testing set:

```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

2. Instantiate and train the perceptron on the training set:

```
from sklearn.linear_model import Perceptron

pr = Perceptron()
pr.fit(X_train_scaled, y_train)

Perceptron(alpha=0.0001, class_weight=None, eta0=1.0,
fit_intercept=True,
n_iter=5, n_jobs=1, penalty=None, random_state=0, shuffle=True,
verbose=0, warm_start=False)
```

3. Measure the cross-validation score. Pass `roc_auc` as the cross-validation scoring mechanism. Additionally, use a stratified k-fold by setting `cv=skf`:

```
from sklearn.model_selection import cross_val_score,
StratifiedKFold

skf = StratifiedKFold(n_splits=3)
cross_val_score(pr, X_train_scaled, y_train,
cv=skf, scoring='roc_auc').mean()

0.76832628835771022
```

4. Measure the performance on the test set. Import two metrics, `accuracy_score` and `roc_auc_score`, from the `sklearn.metrics` module:

```
from sklearn.metrics import accuracy_score, roc_auc_score

print "Classification accuracy : ", accuracy_score(y_test,
pr.predict(X_test_scaled))
print "ROC-AUC Score : ", roc_auc_score(y_test,
pr.predict(X_test_scaled))
```

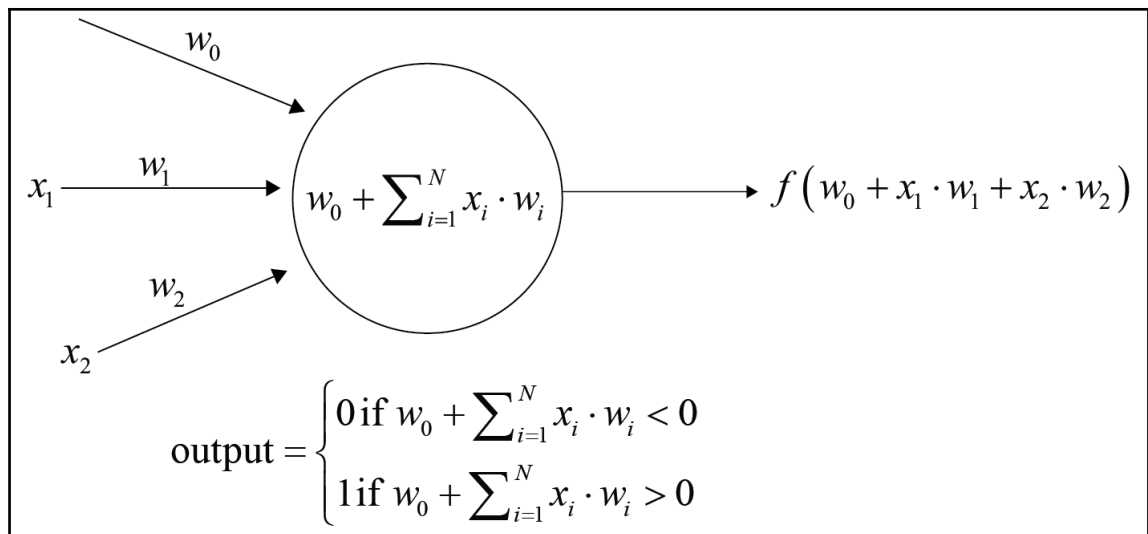
Classification accuracy : 0.681818181818
ROC-AUC Score : 0.682592592593

The test finished relatively quickly. It performed okay, a bit worse than logistic regression, which was 75% accurate (this is an estimate; we cannot compare the logistic regression from any previous chapter because the training/testing split is different).

How it works...

The perceptron is a simplification of a neuron in the brain. In the following diagram, the perceptron receives inputs x_1 and x_2 from the left. A bias term, w_0 , and weights w_1 and w_2 are computed. The terms x_i and w_i form a linear function. This linear function is then passed to an activation function.

In the following activation function, if the sum of the dot product of the weight and input vector is less than zero, an individual row is classified as 0; otherwise it is classified as 1:



This happens in a single epoch, or iteration, passing through the perceptron. The process repeats through several iterations and weights are readjusted each time, minimizing the loss function.

With regard to perceptrons and the current state of neural networks, they work well as researchers have tried many things. In practice, they currently work well with the computational power available now.

As computing power keeps increasing, neural networks and perceptrons become capable of solving increasingly difficult problems and training times keep decreasing and decreasing.

There's more...

Try running a grid search by varying the perceptron's hyperparameters. Some notable parameters include regularization parameters, `penalty` and `alpha`, `class_weight`, and `max_iter`. The `class_weight` parameter deals well with unbalanced classes by giving more weight to the underrepresented classes. The `max_iter` parameter refers to the maximum number of passes through the perceptron. In general, the higher its value the better, so we set it to 50. (Note that this is the code for scikit-learn 0.19.0. In scikit-learn 0.18.1, use the `n_iter` parameter instead of the `max_iter` parameter.)

Try the following grid search:

```
from sklearn.model_selection import GridSearchCV

param_dist = {'alpha': [0.1,0.01,0.001,0.0001],
              'penalty': [None, 'l2', 'l1', 'elasticnet'],
              'random_state': [7],
              'class_weight': ['balanced',None], 'eta0': [0.25,0.5,0.75,1.0],
              'warm_start':[True,False], 'max_iter':[50], 'tol':[1e-3]}

gs_perceptron = GridSearchCV(pr, param_dist,
                             scoring='roc_auc',cv=skf).fit(X_train_scaled, y_train)
```

Look at the best parameters and the best score:

```
gs_perceptron.best_params_

{'alpha': 0.001,
 'class_weight': None,
 'eta0': 0.5,
 'max_iter': 50,
 'penalty': 'l2',
 'random_state': 7,
 'tol': 0.001,
 'warm_start': True}

gs_perceptron.best_score_
```

0.79221656570311072

Varying hyperparameters using cross-validation has improved the results. Now try to use bagging with a set of perceptrons as follows. Start by noticing and picking the best perceptron from the perceptron grid search:

```
best_perceptron = gs_perceptron.best_estimator_
```

Perform the grid search:

```
from sklearn.ensemble import BaggingClassifier

from sklearn.ensemble import BaggingClassifier
param_dist = {
    'max_samples': [0.5,1.0],
    'max_features' : [0.5,1.0],
    'oob_score' : [True, False],
    'n_estimators': [100],
    'n_jobs': [-1],
    'base_estimator__alpha': [0.001,0.002],
    'base_estimator__penalty': [None, 'l2', 'l1', 'elasticnet'], }

ensemble_estimator = BaggingClassifier(base_estimator = best_perceptron)
bag_perceptrons = GridSearchCV(ensemble_estimator,
    param_dist,scoring='roc_auc',cv=skf,n_jobs=-1).fit(X_train_scaled, y_train)
```

Look at the new cross-validation score and best parameters:

```
bag_perceptrons.best_score_

0.83299842529587864

bag_perceptrons.best_params_

{'base_estimator__alpha': 0.001,
 'base_estimator__penalty': 'l1',
 'max_features': 1.0,
 'max_samples': 1.0,
 'n_estimators': 100,
 'n_jobs': -1,
 'oob_score': True}
```

Thus, a bag of perceptrons scores better than a single perceptron for this dataset.

Neural network – multilayer perceptron

Using a neural network in scikit-learn is straightforward and proceeds as follows:

1. Load the data.
2. Scale the data with a standard scaler.
3. Do a hyperparameter search. Begin by varying the alpha parameter.

Getting ready

Load the medium-sized California housing dataset that we used in *Chapter 9, Tree Algorithms and Ensembles*:

```
%matplotlib inline

import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import fetch_california_housing

cali_housing = fetch_california_housing()

X = cali_housing.data
y = cali_housing.target
```

Bin the target variable so that the target train set and target test set are a bit more similar. Then use a stratified train/test split:

```
bins = np.arange(6)
binned_y = np.digitize(y, bins)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.2, stratify=binned_y)
```

How to do it...

1. Begin by scaling the input variables. Train the scaler only on the training data:

```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler()
scaler.fit(X_train)

X_train_scaled = scaler.transform(X_train)
```

2. Then, perform the scaling on the test set:

```
X_test_scaled = scaler.transform(X_test)
```

3. Finally, perform a randomized search (or grid search if you prefer) to find a reasonable value for `alpha`, one that scores well:

```
from sklearn.model_selection import RandomizedSearchCV
from sklearn.neural_network import MLPRegressor

param_grid = {'alpha': [10, 1, 0.1, 0.01],
              'hidden_layer_sizes' :
                [(50, 50, 50), (50, 50, 50, 50, 50)],
              'activation': ['relu', 'logistic'],
              'solver' : ['adam']}

pre_gs_inst = RandomizedSearchCV(MLPRegressor(random_state=7),
                                param_distributions = param_grid,
                                cv=3,
                                n_iter=15,
                                random_state=7)
pre_gs_inst.fit(X_train_scaled, y_train)

pre_gs_inst.best_score_

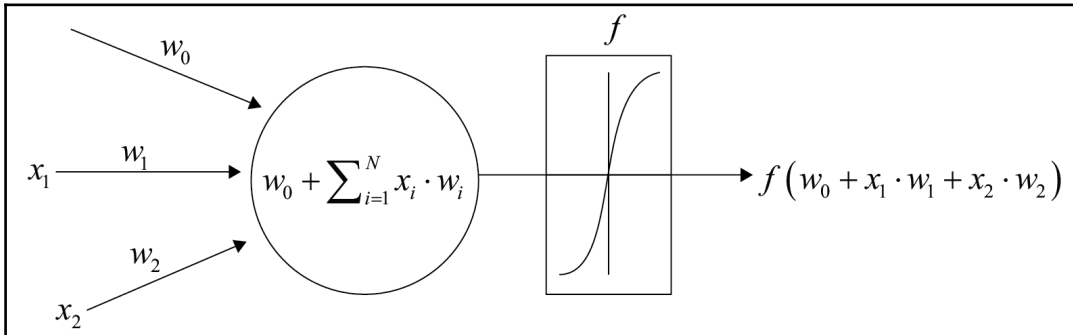
0.7729679848718175

pre_gs_inst.best_params_

{'activation': 'relu',
 'alpha': 0.01,
 'hidden_layer_sizes': (50, 50, 50),
 'solver': 'adam'}
```

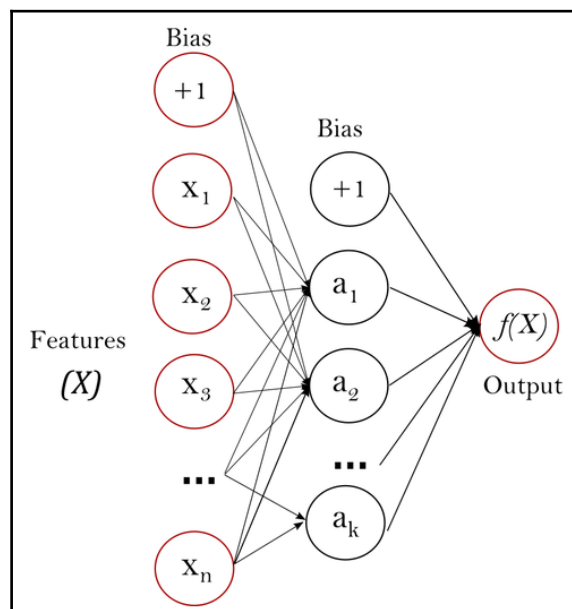
How it works...

In the context of neural networks, the single perceptrons look like this:



The output is a function of a sum of the dot product of weights and inputs. The function f is the activation function and can be a sigmoid curve, for example. In the neural network, hyperparameter activation refers to this function. In scikit-learn, there are the options of identity, logistic, tanh, and relu, where logistic is the sigmoid curve.

The whole network looks like this (the following is a diagram from the scikit documentation at http://scikit-learn.org/stable/modules/neural_networks_supervised.html):



It is instructive to use a neural network on a dataset we are familiar with, the California housing dataset. The California housing dataset seemed to favor nonlinear algorithms, particularly trees and ensembles of trees. Trees did well on the dataset and established a benchmark as to how well algorithms can do on that dataset.

In the end, neural networks did okay but not nearly as well as gradient boosting machines. Additionally, they were computationally expensive.

Philosophical thoughts on neural networks

Neural networks are mathematically universal function approximators and can learn any function. Also, the hidden layers are often interpreted as the network learning the intermediate steps of a process without a human having to program the intermediate steps. This can come from convolutional neural networks in computer vision, where it is easy to see how the neural network figures out each layer.

These facts make an interesting mental image and can be applied to other estimators. Many people do not tend to think of random forests as trees figuring out processes tree level by tree level, or tree by tree (perhaps because their structure is not as organized and random forests do not invoke visualizations of the biological brain). In more practical detail, if you wanted to organize random forests, you can limit their depth or perhaps use gradient boosting machines.

Regardless of the hard facts present or not in the idea of a neural network truly being intelligent, it is helpful to carry around such mental images as the field progresses and machines become smarter and smarter. Carry the idea around, yet focus on the results as they are; that's what machine learning is about now.

Stacking with a neural network

The two most common meta-learning methods are bagging and boosting. Stacking is less widely used; yet it is powerful because one can combine models of different types. All three methods create a stronger estimator from a set of not-so-strong estimators. We tried the stacking procedure in [Chapter 9, *Tree Algorithms and Ensembles*](#). Here, we try it with a neural network mixed with other models.

The process for stacking is as follows:

1. Split the dataset into training and testing sets.
2. Split the training set into two sets.

3. Train base learners on the first part of the training set.
4. Make predictions using the base learners on the second part of the training set. Store these prediction vectors.
5. Take the stored prediction vectors as inputs and the target variable as output. Train a higher level learner (note that we are still on the second part of the training set).

After that, you can view the results of the overall process on the test set (note that you cannot select a model by viewing results on the test set).

Getting ready

Import the California housing dataset and the libraries we have been using: `numpy`, `pandas`, and `matplotlib`. It is a medium-sized dataset but is large relative to the other scikit-learn datasets:

```
from __future__ import division
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.datasets import fetch_california_housing

#From within an ipython notebook
%matplotlib inline

cali_housing = fetch_california_housing()

X = cali_housing.data
y = cali_housing.target
```

Bin the target variable to increase the balance in splitting the dataset in regards to the target:

```
bins = np.arange(6)
binned_y = np.digitize(y, bins)
```

Split the dataset `X` and `y` into three sets. `X_1` and `X_stack` refer to the input variables of the first and second training sets, respectively. `y_1` and `y_stack` refer to the output target variables of the first and second training sets respectively. The test set consists of `X_test_prin` and `y_test_prin`:

```
from sklearn.model_selection import train_test_split
X_train_prin, X_test_prin, y_train_prin, y_test_prin = train_test_split(X,
y, test_size=0.2, stratify=binned_y, random_state=7)
```

```

binned_y_train_prin = np.digitize(y_train_prin, bins)

X_1, X_stack, y_1, y_stack =
train_test_split(X_train_prin, y_train_prin, test_size=0.33, stratify=binned_y
_train_prin, random_state=7 )

```

Another option is to use `StratifiedShuffleSplit` from the `model_selection` module in `scikit-learn`.

How to do it...

We are going to use three base regressors: a neural network, a single gradient boosting machine, and a bag of gradient boosting machines.

First base model – neural network

1. Add a neural network by performing a cross-validated grid search on the first training set: `X_1`, the inputs, and `y_1` the target set. This will find the best parameters of the neural network for this dataset. We are only varying the `alpha` parameter in this example. Do not forget to scale the inputs or else the network will not run well:

```

from sklearn.model_selection import GridSearchCV
from sklearn.neural_network import MLPRegressor

from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

mlp_pipe = Pipeline(steps=[('scale', StandardScaler()),
                           ('neural_net', MLPRegressor())])

param_grid = {'neural_net__alpha': [0.02, 0.01, 0.005],
              'neural_net__hidden_layer_sizes' : [(50, 50, 50)],
              'neural_net__activation': ['relu'],
              'neural_net__solver' : ['adam']}

neural_net_gs = GridSearchCV(mlp_pipe, param_grid =
param_grid, cv=3, n_jobs=-1)
neural_net_gs.fit(X_1, y_1)

```

2. View the best parameters and the best score of the grid search:

```
neural_net_gs.best_params_  
  
{'neural_net__activation': 'relu',  
 'neural_net__alpha': 0.01,  
 'neural_net__hidden_layer_sizes': (50, 50, 50),  
 'neural_net__solver': 'adam'}  
  
neural_net_gs.best_score_  
  
0.77763106799320014
```

3. Pickle the neural network that performed the best during the grid search. This will save the training we have done so that we do not have to keep doing it several times:

```
nn_best = neural_net_gs.best_estimator_  
  
import pickle  
  
f = open('nn_best.save', 'wb')  
pickle.dump(nn_best, f, protocol = pickle.HIGHEST_PROTOCOL)  
f.close()
```

Second base model – gradient boost ensemble

4. Perform a randomized grid search on gradient-boosted trees:

```
from sklearn.model_selection import RandomizedSearchCV  
from sklearn.ensemble import GradientBoostingRegressor  
  
param_grid = {'learning_rate': [0.1, 0.05, 0.03, 0.01],  
              'loss': ['huber'],  
              'max_depth': [5, 7, 10],  
              'max_features': [0.4, 0.6, 0.8, 1.0],  
              'min_samples_leaf': [2, 3, 5],  
              'n_estimators': [100],  
              'warm_start': [True], 'random_state': [7]  
              }  
  
boost_gs = RandomizedSearchCV(GradientBoostingRegressor(),  
param_distributions = param_grid, cv=3, n_jobs=-1, n_iter=25)  
boost_gs.fit(X_1, y_1)
```

5. View the best score and parameters:

```
boost_gs.best_score_

0.82767651150013244

boost_gs.best_params_

{'learning_rate': 0.1, 'loss': 'huber', 'max_depth': 10,
 'max_features': 0.4, 'min_samples_leaf': 5, 'n_estimators': 100,
 'random_state': 7, 'warm_start': True}
```

6. Increase the number of estimators and train:

```
gbt_inst = GradientBoostingRegressor(**{'learning_rate': 0.1,
 'loss': 'huber',
 'max_depth': 10,
 'max_features': 0.4,
 'min_samples_leaf': 5,
 'n_estimators': 4000,
 'warm_start': True, 'random_state': 7}).fit(X_1, y_1)
```

7. Pickle the estimator. For convenience and reusability, the pickling code is wrapped into a single function:

```
def pickle_func(filename, saved_object):
    import pickle

    f = open(filename, 'wb')
    pickle.dump(saved_object, f, protocol =
pickle.HIGHEST_PROTOCOL)
    f.close()
    return None

pickle_func('grad_boost.save', gbt_inst)
```

Third base model – bagging regressor of gradient boost ensembles

8. Now, perform a small grid search for a bag of gradient-boosted trees. It is hard to know from a theoretical viewpoint whether this type of ensemble will do well. For the purpose of stacking, it will do well enough if it is not too correlated with the other base estimators:

```
from sklearn.ensemble import
BaggingRegressor, GradientBoostingRegressor
from sklearn.model_selection import RandomizedSearchCV

param_dist = {
    'max_samples': [0.5, 1.0],
    'max_features' : [0.5, 1.0],
    'oob_score' : [True, False],
    'base_estimator__min_samples_leaf': [4, 5],
    'n_estimators': [20]
}

single_estimator = GradientBoostingRegressor(**{'learning_rate':
0.1,
'loss': 'huber',
'max_depth': 10,
'max_features': 0.4,
'n_estimators': 20,
'warm_start': True, 'random_state': 7})

ensemble_estimator = BaggingRegressor(base_estimator =
single_estimator)

pre_gs_inst_bag = RandomizedSearchCV(ensemble_estimator,
param_distributions = param_dist,
cv=3,
n_iter = 5,
n_jobs=-1)

pre_gs_inst_bag.fit(X_1, y_1)
```

9. View the best parameters and score:

```
pre_gs_inst_bag.best_score_

0.78087218305611195

pre_gs_inst_bag.best_params_

{'base_estimator__min_samples_leaf': 5,
'max_features': 1.0,
'max_samples': 1.0,
'n_estimators': 20,
'oob_score': True}
```

10. Pickle the best estimator:

```
pickle_func('bag_gbm.save', pre_gs_inst_bag.best_estimator_)
```

Some functions of the stacker

11. Use functions similar to Chapter 9, *Tree Algorithms and Ensembles*. The `handle_X_set` function creates a dataframe of the prediction vectors on the `X_stack` set. Conceptually, it refers to the fourth step of predictions on the second part of the training set:

```
def handle_X_set(X_train_set_in):
    X_train_set = X_train_set_in.copy()
    y_pred_nn = neural_net.predict(X_train_set)
    y_pred_gbt = gbt.predict(X_train_set)
    y_pred_bag = bag_gbm.predict(X_train_set)
    preds_df = pd.DataFrame(columns = ['nn', 'gbt', 'bag'])

    preds_df['nn'] = y_pred_nn
    preds_df['gbt'] = y_pred_gbt
    preds_df['bag'] = y_pred_bag

    return preds_df

def predict_from_X_set(X_train_set_in):
    X_train_set = X_train_set_in.copy()
    return final_etr.predict(handle_X_set(X_train_set))
```

12. If you pickled the files previously and want to start at this step, unpickle the files. The following files are loaded with the correct filenames and variable names to perform the `handle_X_set` function:

```
def pickle_load_func(filename):
    f = open(filename, 'rb')
    to_return = pickle.load(f)
    f.close()
    return to_return

neural_net = pickle_load_func('nn_best.save')
gbt = pickle_load_func('grad_boost.save')
bag_gbm = pickle_load_func('bag_gbm.save')
```

13. Create a dataframe of predictions using the `handle_X_set` function. Print the Pearson correlation between the prediction vectors:

```
preds_df = handle_X_set(X_stack)
print (preds_df.corr())
```

	nn	gbt	bag
nn	1.000000	0.867669	0.888655
gbt	0.867669	1.000000	0.981368
bag	0.888655	0.981368	1.000000

Meta-learner – extra trees regressor

14. Similar to Chapter 9, *Tree Algorithms and Ensembles*, train an extra tree regressor on the dataframe of predictions. Use `y_stack` as the target vector:

```
from sklearn.ensemble import ExtraTreesRegressor
from sklearn.model_selection import RandomizedSearchCV

param_dist = {'max_features' : ['sqrt', 'log2', 1.0],
              'min_samples_leaf' : [1, 2, 3, 7, 11],
              'n_estimators': [50, 100],
              'oob_score': [True, False]}

pre_gs_inst =
RandomizedSearchCV(ExtraTreesRegressor(warm_start=True, bootstrap=True,
random_state=7),
                  param_distributions = param_dist,
                  cv=3,
                  n_iter = 15, random_state=7)

pre_gs_inst.fit(preds_df.values, y_stack)
```

15. View the best parameters:

```
pre_gs_inst.best_params_

{'max_features': 1.0,
 'min_samples_leaf': 11,
 'n_estimators': 100,
 'oob_score': False}
```

16. Train the extra trees regressor but increase the number of estimators:

```
final_etr = ExtraTreesRegressor(**{'max_features': 1.0,
    'min_samples_leaf': 11,
    'n_estimators': 3000,
    'oob_score': False, 'random_state': 7}).fit(preds_df.values,
    y_stack)
```

17. View the `final_etr` estimator's cross-validation performance:

```
from sklearn.model_selection import cross_val_score

cross_val_score(final_etr, preds_df.values, y_stack, cv=3).mean()

0.82212054913537747
```

18. View the performance on the testing set:

```
y_pred = predict_from_X_set(X_test_prin)

from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_test_prin, y_pred)
print "MAE : ", mean_absolute_error(y_test_prin, y_pred)
print "MAPE : ", (np.abs(y_test_prin- y_pred)/y_test_prin).mean()

R-squared 0.839538887753
MAE : 0.303109168851
MAPE : 0.168643891048
```

19. Perhaps we can increase the results even further. Place the training columns alongside the prediction vectors. Start by modifying the functions we have been using:

```
def handle_X_set_sp(X_train_set_in):
    X_train_set = X_train_set_in.copy()
    y_pred_nn = neural_net.predict(X_train_set)
    y_pred_gbt = gbt.predict(X_train_set)
    y_pred_bag = bag_gbm.predict(X_train_set)
    #only change in function: include input vectors in training
    dataframe
    preds_df = pd.DataFrame(X_train_set, columns =
    cali_housing.feature_names)
    preds_df['nn'] = y_pred_nn
    preds_df['gbt'] = y_pred_gbt
    preds_df['bag'] = y_pred_bag
```



```

        return preds_df

def predict_from_X_set_sp(X_train_set_in):
    X_train_set = X_train_set_in.copy()

    #change final estimator's name to final_etr_sp and use
    handle_X_set_sp within this function
    return final_etr_sp.predict(handle_X_set_sp(X_train_set))

```

20. Continue the training of the extra trees regressor as before:

```

preds_df_sp = handle_X_set_sp(X_stack)

from sklearn.ensemble import ExtraTreesRegressor
from sklearn.model_selection import RandomizedSearchCV

param_dist = {'max_features' : ['sqrt', 'log2', 1.0],
              'min_samples_leaf' : [1, 2, 3, 7, 11],
              'n_estimators': [50, 100],
              'oob_score': [True, False]}

pre_gs_inst_2 =
RandomizedSearchCV(ExtraTreesRegressor(warm_start=True, bootstrap=True,
random_state=7),
    param_distributions = param_dist,
    cv=3,
    n_iter = 15, random_state=7)

pre_gs_inst_2.fit(preds_df_sp.values, y_stack)

```

21. We continue as we did previously. View the best parameters and train a model with more estimators:

```

{'max_features': 'log2',
 'min_samples_leaf': 2,
 'n_estimators': 100,
 'oob_score': False}

final_etr_sp = ExtraTreesRegressor(**{'max_features': 'log2',
    'min_samples_leaf': 2,
    'n_estimators': 3000,
    'oob_score': False, 'random_state': 7}).fit(preds_df_sp.values,
y_stack)

```

22. View cross-validation performance:

```
from sklearn.model_selection import cross_val_score

cross_val_score(final_etf_sp, preds_df_sp.values, y_stack,
cv=3).mean()

0.82978653642597144
```

23. We included the original input columns in the training of the high-level learner of the stacker. The cross-validation performance has increased to 0.8297 from 0.8221. Thus, we conclude that the model that includes the input columns is the best model. Now, after we have selected this model as the final best model, we look at the performance of the estimator on the testing set:

```
y_pred = predict_from_X_set_sp(X_test_prin)

from sklearn.metrics import r2_score, mean_absolute_error

print "R-squared", r2_score(y_test_prin, y_pred)
print "MAE : ", mean_absolute_error(y_test_prin, y_pred)
print "MAPE : ", (np.abs(y_test_prin- y_pred)/y_test_prin).mean()

R-squared 0.846455829258
MAE : 0.295381654368
MAPE : 0.163374936923
```

There's more...

After trying out neural networks on scikit-learn, you can try packages such as *skflow*, which borrows the syntax of scikit-learn yet utilizes Google's powerful open source TensorFlow.

In regards to stacking, you can try cross-validation performance and prediction on the whole training set *X_train_prin*, instead of splitting it into two parts, *X_1* and *X_stack*.

A lot of packages in data science borrow heavily from either scikit-learn's or R's syntaxes.

12

Create a Simple Estimator

In this chapter we will cover the following recipes:

- Creating a simple estimator

Introduction

We are going to make a custom estimator with scikit-learn. We will take traditional statistical math and programming and turn it into machine learning. You are able to turn any statistics into machine learning by using scikit-learn's powerful cross-validation capabilities.

Create a simple estimator

We are going to do some work towards building our own scikit-learn estimator. The custom scikit-learn estimator consists of at least three methods:

- An `__init__` initialization method: This method takes as input the estimator's parameters
- A `fit` method: This trains the estimator
- A `predict` method: This method performs a prediction on unseen data

Schematically, the class looks like this:

```
#Inherit from the classes BaseEstimator, ClassifierMixin
class RidgeClassifier(BaseEstimator, ClassifierMixin):

    def __init__(self, param1, param2):
        self.param1 = param1
        self.param2 = param2

    def fit(self, X, y = None):
        #do as much work as possible in this method
        return self

    def predict(self, X_test):
        #do some work here and return the predictions, y_pred
        return y_pred
```

Getting ready

Load the breast cancer dataset from scikit learn:

```
import numpy as np
import pandas as pd

from sklearn.datasets import load_breast_cancer

bc = load_breast_cancer()

new_feature_names = ['_'.join(ele.split()) for ele in bc.feature_names]

X = pd.DataFrame(bc.data, columns = new_feature_names)
y = bc.target
```

Split the data into training and testing sets:

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33,
random_state=7, stratify = y)
```

How to do it...

A scikit estimator should have a `fit` method, that returns the class itself, and a `predict` method, that returns the predictions:

1. The following is a classifier we call `RidgeClassifier`. Import `BaseEstimator` and `ClassifierMixin` from `sklearn.base` and pass them along as arguments to your new classifier:

```
from sklearn.base import BaseEstimator, ClassifierMixin
from sklearn.linear_model import Ridge

class RidgeClassifier(BaseEstimator, ClassifierMixin):
    """A Classifier made from Ridge Regression"""
    def __init__(self, alpha=0):
        self.alpha = alpha
    def fit(self, X, y = None):
        #pass along the alpha parameter to the internal ridge
        estimator and perform a fit using it
        self.ridge_regressor = Ridge(alpha = self.alpha)
        self.ridge_regressor.fit(X, y)
        #save the seen class labels
        self.class_labels = np.unique(y)
        return self
    def predict(self, X_test):
        #store the results of the internal ridge regressor
        estimator
        results = self.ridge_regressor.predict(X_test)
        #find the nearest class label
        return np.array([self.class_labels[np.abs(self.class_labels
        - x).argmin()] for x in results])
```

Let's focus on the `__init__` method. There, we input a single parameter; it corresponds to the regularization parameter in the underlying ridge regressor.

In the `fit` method, we perform all of the work. The work consists of using an internal ridge regressor and storing the class labels within the data. We might want to throw an error if there are more than two classes, as many classes usually do not map well to a set of real numbers. In this example, there are two possible targets: malignant cancer or benign cancer. They map to real numbers as the degree of malignancy, which can be viewed as diametrically opposed to benignness. In the iris dataset, there are Setosa, Versicolor, and Virginica flowers. The Setosanness quality does not have a guaranteed diametric opposite except looking at the classifier in a one-versus-rest manner.

In the `predict` method, you find the class label that is closest to what the ridge regressor predicts.

2. Now write a few lines applying your new ridge classifier:

```
r_classifier = RidgeClassifier(1.5)
r_classifier.fit(X_train, y_train)
r_classifier.score(X_test, y_test)

0.95744680851063835
```

3. It scores pretty well on the test set. You can perform a grid search on it as well:

```
from sklearn.model_selection import GridSearchCV

param_grid = {'alpha': [0, 0.5, 1.0, 1.5, 2.0]}
gs_rc = GridSearchCV(RidgeClassifier(), param_grid, cv =
3).fit(X_train, y_train)

gs_rc.grid_scores_

[mean: 0.94751, std: 0.00399, params: {'alpha': 0},
 mean: 0.95801, std: 0.01010, params: {'alpha': 0.5},
 mean: 0.96063, std: 0.01140, params: {'alpha': 1.0},
 mean: 0.96063, std: 0.01140, params: {'alpha': 1.5},
 mean: 0.96063, std: 0.01140, params: {'alpha': 2.0}]
```

How it works...

The point of making your own estimator is that the estimator inherits properties from the scikit-learn base estimator and classifier classes. In the line:

```
r_classifier.score(X_test, y_test)
```

Your classifier looked at the default accuracy score for all scikit-learn classifiers. Conveniently, you did not have to look it up or implement it. Besides, when it came to using your classifier, the procedure was very similar to using any scikit classifier.

In the following example, we use a logistic regression classifier:

```
from sklearn.linear_model import LogisticRegression

lr = LogisticRegression()
lr.fit(X_train,y_train)
lr.score(X_test,y_test)

0.9521276595744681
```



Your new classifier did slightly better than logistic regression.

There's more...

At times, statistical packages such as Python's `statsmodels` or `rpy` (an interface to R within Python) contain very interesting statistical methods and you would want to pass them through scikit's cross-validation. Alternatively, you could have written the method and would like to cross-validate it.

The following is a custom estimator constructed using the `statsmodels` **general estimating equation (GEE)** available at <http://www.statsmodels.org/dev/gee.html>.

The GEEs use general linear models (that borrow from R) and we can choose a group-like variable where observations are possibly correlated within a cluster but uncorrelated across clusters—in the words of the documentation. Thus we can group, or cluster, by some variable and see within-group correlations.

Here, we create a model from the breast cancer data based on the R-style formula:

```
'y ~ mean_radius + mean_texture + mean_perimeter + mean_area +
mean_smoothness + mean_compactness + mean_concavity + mean_concave_points +
mean_symmetry + mean_fractal_dimension + radius_error + texture_error +
perimeter_error + area_error + smoothness_error + compactness_error +
concavity_error + concave_points_error + symmetry_error +
fractal_dimension_error + worst_radius + worst_texture + worst_perimeter +
worst_area + worst_smoothness + worst_compactness + worst_concavity +
worst_concave_points + worst_symmetry + worst_fractal_dimension'
```

We cluster by the feature `mean_concavity` (the variable `mean_concavity` is not included in the R-style formula). Start by importing the `statsmodels` module's libraries. The example is as follows:

```
import statsmodels.api as sm
import statsmodels.formula.api as smf

from sklearn.base import BaseEstimator, ClassifierMixin

from sklearn.linear_model import Ridge

class GEEClassifier(BaseEstimator, ClassifierMixin):
    """A Classifier made from statsmodels' Generalized Estimating Equations
    documentation available at: http://www.statsmodels.org/dev/gee.html
    """
    def __init__(self, group_by_feature):
        self.group_by_feature = group_by_feature
    def fit(self, X, y = None):
        #Same settings as the documentation's example:
        self.fam = sm.families.Poisson()
        self.ind = sm.cov_struct.Exchangeable()
        #Auxiliary function: only used in this method within the class
        def expand_X(X, y, desired_group):
            X_plus = X.copy()
            X_plus['y'] = y
            #roughly make ten groups
            X_plus[desired_group + '_group'] = (X_plus[desired_group] *
10) // 10
            return X_plus
        #save the seen class labels
        self.class_labels = np.unique(y)
        dataframe_feature_names = X.columns
        not_group_by_features = [x for x in dataframe_feature_names if x !=
self.group_by_feature]
        formula_in = 'y ~ ' + ' + '.join(not_group_by_features)
        data = expand_X(X, y, self.group_by_feature)
        self.mod = smf.gee(formula_in,
                           self.group_by_feature + "_group",
                           data,
                           cov_struct=self.ind,
                           family=self.fam)
        self.res = self.mod.fit()
        return self
    def predict(self, X_test):
        #store the results of the internal GEE regressor estimator
        results = self.res.predict(X_test)
        #find the nearest class label
```



```

        return np.array([self.class_labels[np.abs(self.class_labels -
x).argmin()]] for x in results])
    def print_fit_summary(self):
        print res.summary()
        return self

```

The code within the `fit` method is similar to the code within the GEE documentation. You can work it out for your particular situation or statistical method. The code within the `predict` method is similar to the ridge classifier you created.

If you run the code like you did for the ridge estimator:

```

gee_classifier = GEEClassifier('mean_concavity')
gee_classifier.fit(X_train, y_train)
gee_classifier.score(X_test, y_test)

0.94680851063829785

```

The point is that you turned a traditional statistical method into a machine learning method using scikit-learn's cross-validation.

Trying the new GEE classifier on the Pima diabetes dataset

Try the GEE classifier on the Pima diabetes dataset. Load the dataset:

```

import pandas as pd

data_web_address =
"https://archive.ics.uci.edu/ml/machine-learning-databases/pima-indians-dia
betes/pima-indians-diabetes.data"

column_names = ['pregnancy_x',
                'plasma_con',
                'blood_pressure',
                'skin_mm',
                'insulin',
                'bmi',
                'pedigree_func',
                'age',
                'target']

feature_names = column_names[:-1]
all_data = pd.read_csv(data_web_address , names=column_names)

import numpy as np

```

```
import pandas as pd

X = all_data[feature_names]
y = all_data['target']
```

Split the dataset into training and testing:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,
random_state=7, stratify=y)
```

Predict by using the GEE classifier. We will use the `blood_pressure` column as the column to group by:

```
gee_classifier = GEEClassifier('blood_pressure')
gee_classifier.fit(X_train, y_train)
gee_classifier.score(X_test, y_test)

0.80519480519480524
```

You can also try the ridge classifier:

```
r_classifier = RidgeClassifier()
r_classifier.fit(X_train, y_train)
r_classifier.score(X_test, y_test)

0.76623376623376627
```

You can compare these—the ridge classifier and GEE classifier—with logistic regression in the Chapter 5, *Linear Models – Logistic Regression*.

Saving your trained estimator

Saving your custom estimator is the same as saving any scikit-learn estimator. Save the trained ridge classifier in the file `rc_inst.save` as follows:

```
import pickle

f = open('rc_inst.save', 'wb')
pickle.dump(r_classifier, f, protocol = pickle.HIGHEST_PROTOCOL)
f.close()
```

To retrieve the trained classifier and use it, do this:

```
import pickle

f = open('rc_inst.save', 'rb')
r_classifier = pickle.load(f)
f.close()
```

It is very simple to save a trained custom estimator in scikit-learn.

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